

SPECTRAL AND TEMPORAL CHARACTERIZATION OF HIGH-TEMPERATURE EVENTS

THESIS

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AFIT-GAP-ENP-01M-01

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William Bagby

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Abstract

The remote observations of the temporal and spectral characteristics of the infrared (IR) emissions from exploding ordnance have been correlated with explosion conditions. A Bomem MR-154 Fourier Transform Interferometer with two detectors, InSb and HgCdTe, was used to record spectra in the 1.3 - 20 µm range. Data was collected at spectral resolutions of 16 cm⁻¹ and 4 cm⁻¹, and temporal resolutions of 0.045 s and 0.123 s, respectively. The data files range in size from 900 Kilobytes to several Megabytes. These are reduced to 2-dimensional representations of temporal features that are less than 100 Kilobytes.

The data collected from efforts indicate the possibility of characterizing event species through one or more derived temporal features. Each event data matrix contains three dimensions of information describing radiance as a function of frequency and time. The observed data is first corrected for atmospheric losses to convert apparent radiance to emitted radiance. The data is then adjusted to remove background radiance. Finally, the corrected data is fit to a Planckian distribution function to compute event temperature and fractional field of view. Temporal profiles of temperature and fractional field of view are created to describe each event. The temporal profiles of each explosive type are compared to other explosive types. Certain explosive types indicate an afterburn feature on their temperature profiles. The afterburn feature wasn't apparent on the temperature profiles of other types. Additionally, the temporal evolution of fractional field of view was unique for each explosive type.

I. Introduction

Overview

NASA defines remote sensing as, "The acquisition and measurement of data/information on some property(ies) of a phenomenon, object, or material by a recording device not in physical, intimate contact with the feature(s) under surveillance; techniques involve amassing knowledge pertinent to environments by measuring force fields, electromagnetic radiation, or acoustic energy employing cameras, radiometers and scanners, lasers, radio frequency receivers, radar systems, sonar, thermal devices, seismographs, magnetometers, gravimeters, scintillometers, and other instruments." (22, 2-4). By this definition, remote sensing can be as simple as the human eye sensing the reflected light from this text as it is being read or as complicated as satellite measurements of distant parts of the universe. As technology has grown, so have the opportunities for ways to use remote sensing. No longer is remote sensing limited to the visual portion of the electromagnetic spectrum. Today radiation can be captured and recorded from short wavelength x-rays, through visual and infrared, and beyond to longer wavelength radio waves. Each spectral range can be used to detect unique information about unknown objects or events. For example: X-rays detect solar flares, visual photographs provide military intelligence or pictures for disaster relief, infrared determines agricultural crop conditions as well as theater missile defense, and radio waves monitor changing conditions in the polar icecaps. Remote sensing has been used in various applications including medical diagnostics, weather satellite imagery, terrain mapping of Mars, to identifying groceries in the supermarket using barcode scanners.

Remote sensing is widely used in the Department of Defense (DOD). One of the first uses of remote sensing by the US Army Air Corps was photographing troop movements in WWI. The DOD now uses sensing techniques for battlefield management, battle-space characterization, weapons guidance, technical intelligence and threat identification. Today, remote sensing is not limited to visual pictures of troop movements, but includes sensing most of the electromagnetic spectrum. Certain regions of the spectrum provide information about distinct events not apparent in other regions of the spectrum.

This thesis continues the work of Orson (17), "Collection of Detonation signatures and Characterization of Spectral Features". His research focused on the infrared collection of electromagnetic signatures from fifty-six detonation events. These events were collected over the spectral range of 500 to 6000 wavenumbers (cm⁻¹) with .047 seconds time resolution. Collection was accomplished with a Bomem MR-154 Fourier Transform Infrared spectroradiometer. These events were a combination of dynamic F-18 delivered ordnance as well as static detonations. The research was part of infrared Measurement and Signals Intelligence (MASINT) detection of explosions. This MASNIT research is part of a cooperative effort between the Navy Tactical Exploitation of National Capabilities (TENCAP) office and the National Air Intelligence Center's Cobra Brass program office (NAIC/DXDI). This program has sponsored a series of tests where ordinance was detonated under field conditions. These efforts explore the potential use of space-based MASINT sensors to support combat units in the area of Battle-Space Characterization.

The source of detonation data is from munitions detonations performed during the Navy TENCAP sponsored testing of munitions. This series of tests was named Radiant Brass. This series consisted of five tests conducted at the Navel Air Station, (NAS) Fallon, NV. Testing started in June 1998 and was completed October 1999. Throughout the program various contractors and government agencies have supported Radiant Brass by deploying sensors to the test sight collecting event signatures. The primary data requirements for these collection teams were radiometric in nature. For these tests, spectral information was a secondary objective.

Blackbody Radiation and Atmospheric Transmittance

A unique opportunity for remote sensing exists in the InfraRed (IR) portion of the electromagnetic spectrum. Within the IR portion of the spectrum are the peak intensities of radiation from emitters including 300 Kelvin to thousands of degrees Kelvin. The temperature of a graybody can be related to the spectral radiation emitted by an event via Equation 1.1, the Planck Distribution:

$$S(\lambda) = \varepsilon(\lambda) \frac{2\pi hc^2}{\lambda^5} \frac{1}{e^{ch/\lambda kT} - 1}$$
 (1.1)

where

 $S(\lambda)$ = Spectral Radiance as a function of wavelength

 $\varepsilon(\lambda)$ = emissivity as a function of wavelength

 λ = radiation wavelength

 $h = Planck's constant = 6.626 * 10^{-34} W sec^2$

T = absolute temperature in Kelvin

 $c = velocity of light = 2.9979 * 10^8 m/sec$

 $k = Boltzmann's constant = 1.38 * 10^{-23} W sec/K$

The wavelength of maximum emittance (λ_m) in microns is given by,

$$\lambda_{\rm m} = a/T \tag{1.2}$$

A simplified form for total emittance (M), of the Planck distribution are given by the Stefan-Boltzmann Law:

$$M = \sigma T^4 \tag{1.3}$$

where

$$\sigma = \text{constant} = 5.669 * 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$$

If $\varepsilon(\lambda) = 1$, Equation 1.1 describes the radiation emitted from a black body. When $\varepsilon \neq 1$, but is constant, the output from Equation 1.1 is a called a 'gray' body. When $\varepsilon \neq 1$ and is wavelength dependant, it is described as a selective radiator.

Many texts and examples of spectrum use wavelength as its unit of length measurement. In spectroscopic discussions, frequency in the form of wavenumber is more commonly used. The conversion between wavenumber, ν , and wavelength, λ , is:

$$\lambda(\mu m) = \left(\frac{10000}{v(cm^{-1})}\right) \tag{1.4}$$

Since the spectroradiometer software outputs all information in cm⁻¹, these units will be used primarily in this thesis. It is important to note that the wavelength to wavenumber conversion is not linear in wavelength. This changes the shape of the Planckian curve. Higher wavenumber equates to lower wavelength and the wavelength unit of measure trends in the opposite direction. The Planck Distribution function as a function of wavenumber becomes:

$$S(v) = \varepsilon(v) \frac{2hc^2v^3}{e^{chv/kT} - 1}$$
(1.5)

Figure 1.1 shows the shapes and relative intensity of spectral radiance of black bodies at different temperatures. The Figure shows four temperatures; 500, 700, 900 and 1100 degrees Kelvin.

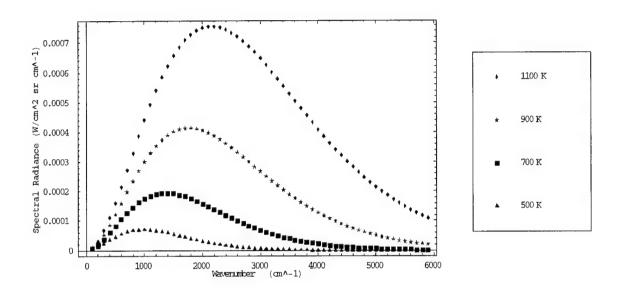


Figure 1.1 Spectral Radiance vs. wavenumber

Also within the IR region of the spectrum there are "transparent" areas where the atmosphere does not significantly absorb electromagnetic radiation and "opaque" regions where energy at a given frequency will be largely absorbed. Phillips Laboratory Expert User Software (PLEXUS) from the Mission Research Corporation (MRC) was used to create atmospheric transmittance profiles. PLEXUS is a knowledge-based, highly user-oriented software platform that integrates and widens the accessibility of the Air Force Research Laboratory (AFRL) family of atmospheric and astronomical background codes. PLEXUS provides an intelligent, intuitive, graphical environment for setting up and running the AFRL Codes and analyzing their output. The AFRL atmospheric codes are the DoD standard models for computing the spectral radiance and transmittance in various regions of the atmosphere. The atmospheric and celestial codes in PLEXUS are

official releases by AFRL. MODerate TRANsmission (MODTRAN) was the AFRL atmospheric model used in PLEXUS for this research. MODTRAN code models the transmission and radiance generally applicable below an altitude of 50 km.

Transmittance is used to describe the portion of source electromagnetic radiation received at the detector after traveling through a given path. Transmittance is a unitless number ranging from zero to one. A value of one represents no signal loss and a value of zero represents a total loss of signal between the source and the detector.

Figure 1.2 shows a PLEXUS/MODTRAN transmittance profile of the atmosphere as a function of wavenumbers. The transmittance profile shown in Figure 1.2 represents the portion of electromagnetic energy that passes between a sensor and a detonation event two miles away. The profile shown in Figure 1.2 was created using the atmospheric conditions recorded at Fallon NAS during testing. The profile represents a 4200 meter line of sight path through the atmosphere 10 meters above the ground. Figure 1.2 has a spectral resolution of 4 cm⁻¹. The frequencies with values of zero are where the atmosphere has completely absorbed the radiation at that frequency. The primary absorbers in the IR are H₂O and CO₂. Figure 1.2 also shows which molecular species is primarily responsible for absorption in opaque frequency intervals. There are also areas where the atmospheric transmittance is close to one. In these frequencies, the radiation received by the detector is in the atmospheric and spatial conditions used is nearly the same as the radiation detected if there were no atmosphere. Theoretically, these frequencies represent where the data is most accurate.

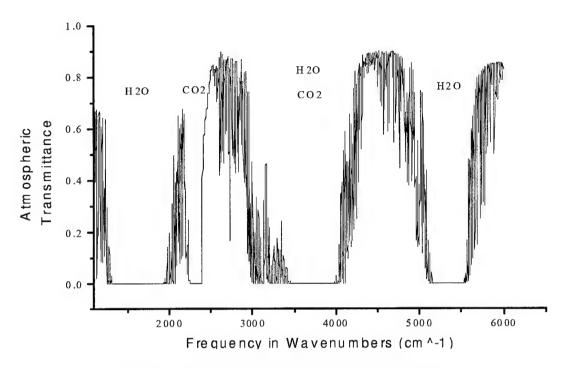


Figure 1.2 Atmospheric Transmittance Profile

By multiplying the transmittance profile by a Planckian blackbody curve at a given temperature, an expected spectral signal can be created. Consider the 1100 Kelvin curve from Figure 1.1 traveling through the atmosphere to our detector. Figure 1.3 represents what an 1100 Kelvin blackbody would be for the atmospheric and spatial conditions used to create the Figure 1.2 transmittance profile. The detector would intercept this signal if the blackbody completely fills the detector's field of view. However, the detector can be calibrated and amplify the signal to approximate the expected event as discussed in chapter II. Figure 1.3 is created by multiplying the unitless numerical value of the transmittance by the intensity value of a blackbody at a given temperature for each frequency value.

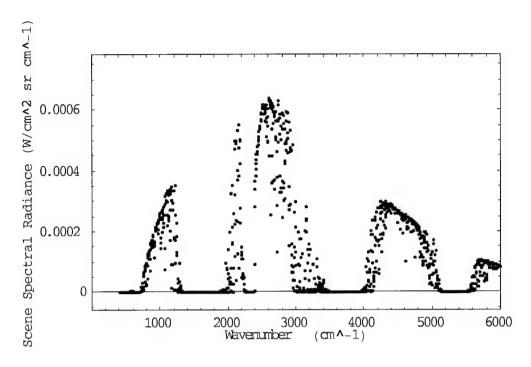


Figure 1.3 1100 Kelvin Intensity with Atmospheric Transmittance

This predicted signal can compared to actual data from one time-step just after bomb detonation in Figure 1.4 shown below.

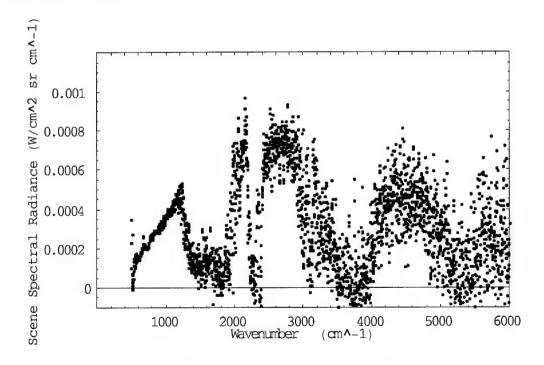


Figure 1.4 Raw Data for One Time Step

Figure 1.4 represents the spectral signal at one time interval within our total data set. In this case, the spectral profile at a time interval just milliseconds after detonation is shown to approximate an 1100 Kelvin blackbody profile. The goal of this research will be to interrogate each time step and identify a pattern for the entire data set. To do this it is important to understand what is expected from the observed event. Since this thesis evaluates the bomb detonation data from the Radiant Brass tests, a quick discussion on explosion mechanistics is necessary.

Explosion Mechanistics

A detonation produces three primary 'sensed' features, an explosion initiation, a secondary afterburn, and a decay period (Cooper, 133). The explosion initiation is caused by the nearly instantaneous conversion of the explosive from chemical potential energy to kinetic energy. The time scale of this feature is less than 1 μ s.

The afterburn feature is the result of the residual products of the detonation. In an under oxidized explosion these residuals are themselves fuels. After the initial pressure pulse of the explosion reaches equilibrium pressure with the surrounding environment, oxygen and air remix with the residual explosion by-products. This mixture of oxygen and residual fuel ignites and causes the energetic afterburn fireball. This feature starts milliseconds after the initiation feature and can last for up to a second. The third feature is the decay of the explosion itself. When the afterburn has consumed all the residual fuel, the event decays back to ambient conditions. This decay feature lasts between 1-3 seconds. These three features make up the primary time history of the 'sensed' explosion. Figure 1.5 shows total radiance as a function of time.

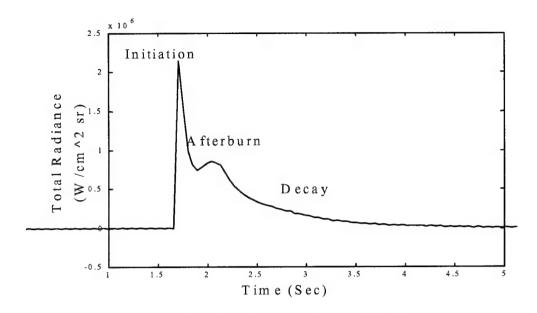


Figure 1.5 Time History of Typical Event

The three features for the event shown in Figure 1.5 are easily distinguished. Explosion initiation occurs at 1.7 seconds, followed by secondary afterburn reaching a peak value at approximately 2.2 seconds then the decay period out to 5 seconds. By assuming that a detonation can be primarily described as a gray body, some general characteristics of a detonation event can be derived. The temperature of a typical explosion initiation feature can be estimated as 1800°K (Cooper, 123). Similarly, the afterburn feature can be estimated as 1100°K, and the decay feature can be estimated as 400°K. By assuming a black body emitter, values for the features of emitted spectra can be predicted. Using Equations 1.2, 1.3, and 1.4, the maximum wavelength, frequency and the total energy of the three temporal features of a typical detonation event can be estimated.

Table 1.1 Predicted Features of Event Emitted Radiation

Feature	Temperature (Kelvin)	Wavelength of Maximum Intensity λ_m (µm)	Total Emittance (W/cm²)
Initiation	1800	1.61	59.50
Afterburn	1100	2.63	8.30
Decay	400	9.66	0.05

Table 1.1 shows expected values for the wavelength of maximum emittance and total emittance of each feature.

Problem Statement

An objective of the Radiant Brass test program is to explore the potential use of space-based MASINT sensors to support combat units in battle-space characterization.

Little infrared spectral information is available on the signatures of conventional weapons. AFIT's collection from the Radiant Brass tests exhibited promise of identification by describing event signatures. The objective of this thesis will be to interpret infrared spectral signatures of detonation events already collected and try to provide some insight into the identification of ordnance or event conditions. In order to accomplish this task a good understanding of the collection process is necessary.

Additionally, an understanding of the data processing procedures is essential. Finally, external variables affecting the event signal collection must be understood. In the case of IR remote sensing, atmospheric absorption is the largest factor affecting signal collection in certain frequencies. Once an atmospheric adjustment is made, then the data is evaluated at each time interval in an effort to find one or more features that can be used for identification of detonation type.

Scope

The focus of the efforts is to determine the feasibility of using the data collected with an FTIR to discriminate high temperature events. This approach will lead to finding one or two features of high temperature events that can be used to describe the event. This thesis begins with the spectral and radiometric data from detonation events collected during previous research. As a feasibility study, some assumptions are made to reach the end results. However, any assumptions will be explained in detail before being applied. Much of the efforts in this research will be on the manipulation of the detonation data and the PLEXUS transmittance data. The two data types are mathematically merged and evaluated together. The data was saved in the American Standard Code for Information Interchange (ASCII) format as *.txt files.

Summary of current knowledge

Orson (17) used AFIT's spectral radiometer to compute the total energy from detonation events. Since there were other agencies collecting data at the detonation events with radiometers, the unique opportunity to compare data was available. Data was integrated in four mostly atmospherically transparent spectral bands to compute an energy total for each band. These four energy totals were then compared to the energy recorded in the same spectral bands using radiometers of other agencies collecting data. This approach was invaluable in verifying the quality of our equipment, procedures and data collected. This work showed that the data collected with our spectral radiometer was within 15% of the radiometer data of other data collection teams. Past research also discussed pattern recognition options for event discrimination and possible future research options. This research will build on previous work and focus on temporal

changes in event temperature and event size for event characterization. Due to the inherent difficulties and costs associated with bomb detonation collection, little spectral data is available on conventional munitions. The analysis in this thesis is limited to the spectral data collected from the Radiant Brass 2A and 2B tests and signatures collected from the Radiant Brass 3A and 3B tests.

The experimental equipment used for collection of the spectral signature data was a Bomem FTIR MR-154 spectrometer. This collection system was comprised of two primary components, the spectrometer itself with its associated optics and the data control computer. The spectrometer was placed on a tripod in clear view of the exploding ordnance. Optics on the front of the spectroradiometer, were used to collect source radiation and help control the system field of view. The field of view of the system was approximately a 300 m diameter circle at 5 km. Two detectors, an Indium Antimonide (InSb) and a Mercury, Cadmium, Telluride (HgCdTe) determined radiance information. A liquid nitrogen dewer attached to the instrument provided a stable cold reference source. A video signal was monitored at the spectroradiometer to improve pointing accuracy. The spectroradiometer was connected to the data control computer by a serial cable. A feed from the instrument optics was placed in the vicinity of the control PC. This video signal was used to provide real time images to the operator and for permanent record on Hi-8 digital tape. All measured signatures were stored on the control PC after each event. The equipment was calibrated on site with a variable temperature black body.

The Bomem *Acquire* software processed the spectral signatures. After proper calibration and data scrubbing the spectrum was saved in ASCII format.

Approach

The primary source of data to be used in this research effort will be the calibrated ASCII data from Radiant Brass 2 and Radiant Brass 3 created during previous research. Since these are very large data files (2200 frequency bins by 250 time bins) up to 12 Megabytes, FORTRAN was used for data manipulation and calculations. Mathematica, MicroCal Origin and Table Curve 2-D were used to verify the results of the FORTRAN output and as display tools.

Locally created atmospheric transmittance files will be used as a partial solution to atmospheric absorption of signal. PLEXUS will be used to 'undo' atmospheric absorption as much as possible to estimate the signal from the source of the emissions.

In addition to the continuation processing data collected during past research, data from various rocket launches were collected as part of this research.

Summary

This completes the introduction material for the collection and analysis of conventional ordnance spectral signatures. Chapter II will provide a discussion of FTIR operations, data manipulation, and fitting procedures used to isolate features of the data. Chapter III will detail the research process step by step. Analysis performed are presented in Chapter IV. Data evaluation results are examined in Chapter V. Finally, Chapter VI will formulate conclusions and offer recommendations for future study.

II. Theory

Introduction

Previous research focused on the remote sensing collection and data verification of various data. This data included detonations of various explosives. Data was collected using AFIT's Bomem FT-154 Fourier Transform Infrared (FTIR) spectroradiometer. The focus of this thesis is to process and interpret the IR emissions collected during previous research.

This chapter will provide the basic theory needed for a reader not familiar with the data collection using the Bomem FT-154 FTIR. The first section will provide an understanding of basic remote sensing principles. The second section will describe the method of information collection, including the FTIR concept of operations, radiance calibration theory and sensor fusion. A review of the sensed object, detonations, will be covered in the bomb phenomenology section. Finally, an in depth discussion of the approach and specific methods used to reach in my research will be discussed.

Since the spectroradiometer software outputs all information in cm⁻¹, these units will be used primarily in this thesis.

Infrared Remote Sensing

The region of the electromagnetic spectrum used for this work is the infrared region. This region of the spectrum is especially well suited for detecting ordnance detonations for three reasons. First, the center frequency of spectral emission is centered in IR region for the afterburn and decay as mentioned in Chapter I and shown in Table 1.1. Second, the IR region provides atmospheric "windows" that allow the signal at

certain frequencies to pass through the atmosphere with little or no loss. Finally, the contrast in emittance between a detonation event and the corresponding IR background is very large. A high contrast allows for easier detection.

Figure 2.1 shows the location of the IR region of the electromagnetic spectrum.

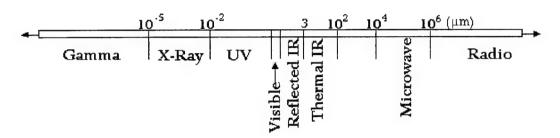
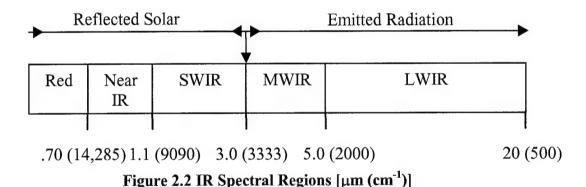


Figure 2.1 Electromagnetic Spectrum

Figure 2.2 shows the location and type of background emission sources as well as many commonly used IR terms.



SWIR stands for Short Wave Infrared while MWIR and LWIR are Mid Wave Infrared and Long Wave Infrared respectively. SWIR is comprised of reflected solar radiation and disappears at night. During the day, the MWIR is a combination of reflected and emitted radiation while at night it is only emitted. The LWIR is always emitted radiation.

By its nature a detonation event is an emitter of radiation. The form and intensity of spectral radiance from a graybody emitter can be produced using Equation 1.1. Since

the amount of energy released in a detonation is large, there's a sharp contrast to the relatively low emittance from the ambient background.

In the discussion of electromagnetic energy emission, propagation and detection, a number of quantities are commonly used. Table 2.1 defines a number of radiometric quantities used to describe the energy content of incoherent radiation fields.

Table 2.1 Radiometric Quantities and Units (21, 14-26)

Quantity	Symbol	Units	Equation	Defining Equation
Radiant energy	Q	Joules	2.1	$Q = \int \Phi dt$
Radiant energy density	W	Joule/cm ³	2.2	$W = \frac{dQ}{dV}$
Radiant flux	Φ	watt	2.3	$\Phi = \frac{dQ}{dt}$
Radiant flux density (Irradiance)	E	watt/m ²	2.4	$E = \frac{d\Phi}{dt}$
Radiant intensity	Ι	watt/str	2.5	$I = \frac{d\Phi}{dt}$
Radiance	L	watt/cm ² str	2.6	$L = \frac{dI}{dA}$

A more detailed description of the spectral and the energy measurement methods performed by the FTIR spectroradiometer will be described in the next section.

Fourier Transform InfraRed (FTIR) Concept of Operation

The detonation data used during this thesis was taken using a Bomem, model MR-154, Fourier Transform Infrared spectroradiometer. Since all data was collected and processed by this instrument, it is important to describe the operation of the equipment in detail.

Many methods for obtaining spectral information rely on the dispersion of light to achieve spectral separation. This is commonly done with a prism or grating. The MR-154 uses a Michelson interferometer to create an interferogram of the input signal. A fourier transform of the interferogram creates the spectra. One advantage of the FTIR technique is all frequencies of the input source are falling on the detector at all times. Figure 2.3 shows the path of the collected IR radiation inside the interferometer.

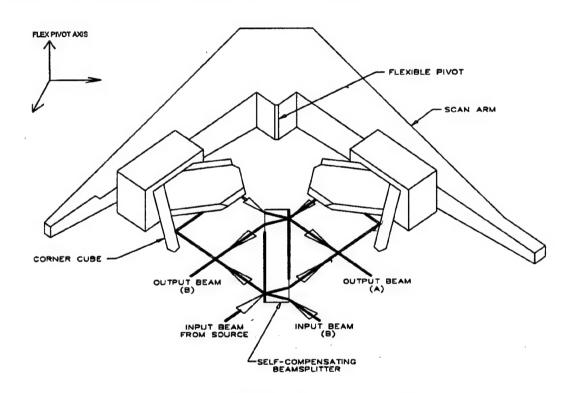


Figure 2.3 MR-154 Scan Arm. (5, 2-5)

The input beam in Figure 2.3 is gathered by the collection optics and collimated by the optics which focus the input beam. Upon striking the beam splitter, the incident beam is split into two different paths. As the scan arm moves, the optical path length changes between the two beams. The two beams are recombined to create constructive and destructive interference patterns based on the differences in the optical path lengths. Generally, intensities for all arm positions in both scan directions are added together to

get one interferogram. These intensities are subsequently decomposed into a spectrum by Fourier transforming the interferogram. In normal operations, one scan of the Michelson interferometer is defined as the forward and reverse sweep of the scan arm. In zero scan mode, a scan is only one sweep direction.

The nature of the FTIR collection method provides inherent broadband capability. No optical filtering is used and the spectral bandwidth is dependant on the detector and beam splitter not the system itself. This provides great flexibility as different detectors can be used with different frequency responses. The maximum optical path length difference of the system limits the spectral resolution. Within the system limits, the control computer can make quick resolution changes.

Digitizing of the interferogram requires precise monitoring of the optical path in the interferometer. The MR-154 uses an internal He-Ne laser, 15798 cm⁻¹, to determine the optical path difference feedback for the system (5, 2-6). The laser provides a known reference signal. This reference ensures very stable optical path length measurements. A liquid nitrogen cold reference source is attached to the MR-154 for an accurate cold body reference. Determining absolute intensity information is a function of the cold reference source, choice of detector, and most importantly calibration.

The MR-154 collects radiant energy as a function of frequency. Spectral radiance can be derived from the signal when the detector hardware and software are given good calibrations and input parameters. A properly set up and well-calibrated system provides useful, accurate measurements that represent the emissions from an unknown source.

The Bomem *Acquire* software controls the Bomem MR-154. During operation, one interferogram is collected using the forward and reverse scans of the Michelson

interferometer. Each measurement is a number of interferograms averaged together. The number of interferograms to average is selected by the user. *Acquire* also controls the spectral range of each detector, the number of measurements to be collected, and the time interval between measurements.

The process of creating an accurate measurement of an unknown has two steps, calibration and unknown acquisition. The first step is to create calibration files using known reference sources. A good calibration consists of at least two radiometric reference points. Ideally, the reference points should straddle the anticipated unknown temperature. Each reference point is built with the same user-selected variables used for measurement. A radiometric reference file is created for each reference point. This process is done by the Bomem *Acquire* software package used with the instrument.

The calibration and data collection process is detailed in Figure 2.4

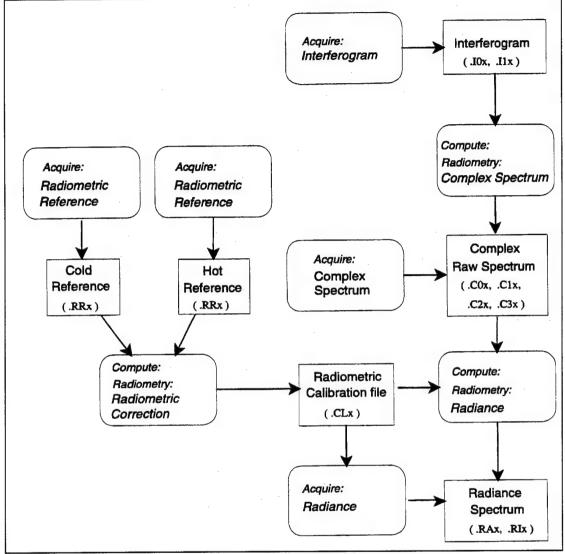


Figure 2.4 Software Measurement Process (5, 7)

The second step to creating accurate measurements from an unknown source is data acquisition. This is accomplished directly in the Acquire software program. The user selects spectral range, number of scans to average per measurement, and number of measurements. The system collects the event data and *Acquire* creates an interferogram file. To process the interferogram, a cosine apodization function is applied. This corrected interferogram is transformed via a Fast Fourier Transform (FFT), to create a

complex raw spectrum file. Applying the radiometric calibration file to the complex raw spectrum file creates the final spectral radiance measurement.

Each block in Figure 2.4 containing a bracketed quantity represents a specific output file from the *Acquire* software. The bracketed quantities refer to the file extension attached to a user-defined filename. An 'x' refers to the detector position, A or B, which is being processed. The *Acquire* software also provides limited data manipulation

Atmospheric effects

Any time electromagnetic energy propagates through the atmosphere, it is affected by atmospheric absorption and scattering. The atmosphere is comprised of many different molecules. Each molecule will absorb different frequencies of electromagnetic radiation due to quantum mechanical interactions. These quantum mechanical interactions include electronic, vibrational and rotational modes of the molecule. Due to relatively low energy levels associated with IR radiation, electronic transitions are not prevalent. The vibrational and rotational modes are the strong absorbing mechanisms. The molecules that absorb electromagnetic radiation in the IR spectrum include H₂0, CO₂, and O₃. Figure 2.5 summarizes the typical vertical atmospheric absorption profile for the Earth atmosphere.

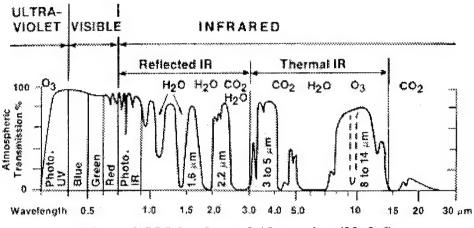


Figure 2.5 Molecules and Absorption (22, 2-6)

 H_2O and CO_2 have many absorption bands. Each large band is related to a vibrational mode. The width of the absorption is due to the rotational modes. The O_3 absorption spectrum around 10 μ m is not an issue for this thesis since O_3 is a minor gas below 100 km in altitude.

Concentrations of H₂O, CO₂, and O₃ are dependent on atmospheric conditions.

These concentrations vary from day to day. The amount of absorption is a function of atmospheric composition and the distance to the source. Atmospheric absorption is commonly described with a transmission coefficient between zero and one. A coefficient of one means no attenuation and coefficients near zero are totally attenuated.

The total attenuation of the atmosphere is a combination of absorption and scattering. Particulates in the atmosphere with radii between 0.1 and 10 μ m attenuate signal between visual and thermal IR frequencies (9, 279). The amount of scattering is based on the particulates cross-sectional area and the frequency of the source radiation. Examples of these particle sources are clouds, smoke, and dust.

Data Manipulation

Data files created from detonation events are very large. Depending on spectral resolution and data collection time, a single file may have as many as 300 temporal steps with up to 2500 frequency steps. FORTRAN was selected for its ability to handle the large data files and manipulate the data efficiently. FORTRAN's strength is in building the data sets into two-dimensional arrays. A 2-D array allows interrogation of the data by timestep or frequency. In building the code, great care was taken to allow for different sizes of data files. It was important to have a program that could determine the size of the data file and read the data regardless of the size or shape of the ASCII file being accessed. The program had to read the ASCII files created from the detonation data and the PLEXUS transmittance profiles. The FORTRAN code was modified to read PLEXUS files and interpolate the value of the transmittance values for the same frequencies as the ASCII data.

Once the interpolation was complete, the ASCII data could be divided by the transmittance value at each frequency to attempt recreation of the signal amplitude at the source. If the PLEXUS value at a given frequency were too small, the adjusted amplitude value at that frequency would be set to zero. Setting the value for adjusted intensity to zero when the transmittance was below a cutoff value had two advantages. First, setting the adjusted value at that frequency to zero avoided overestimated values when dividing by a very small number. Second, if the transmittance is small, the confidence in any signal collected at that frequency would also be small. This method allowed any points with adjusted values of zero to be ignored when fitting to a function.

Mathematica was linked to the FORTRAN program to allow for graphical interface. Mathematica allowed the user to edit the location and filenames of the input ASCII intensity data and PLEXUS transmittance files and the output data files created by FORTRAN. After the program was run, Mathematica could quickly create graphical representations of the data created. The union of Mathematica and FORTRAN proved to be an effective combination of their respective graphical and computational strengths. With the program reading the input files, calculating new values and creating adjusted data files effectively, the identification of temporal features of an event could finally begin.

Data Evaluation

Adjusted intensity data would need to be evaluated for each time step within an event data file. The goal of this evaluation was to find one or two meaningful parameters for each time step that could be followed over the course of the data collection. The evolution of the selected parameters as a function of time were then investigated for identifiable features unique to each type of event. The approach selected was to fit event temperature and size to the Planckian curve representation of two blackbodies. Event size and temperature were adjusted during fitting.

Chapter III will detail the derivation of the equations used to find event temperature and event size. However, an overview of their derivation is necessary prior to a discussion of curve fitting methods used.

The general approach used here will be to assume the signal recorded by the instrument is a result of a single gray body emitter or the combination of two blackbody emitters. The Planck function relates temperature and frequency to the radiation of a

gray body. This function was introduced in chapter I as Equation 1.5 Chapter III will detail the assumption of a black body. The substitution of $\varepsilon(v) = 1$ creates the new form Equation 2.1

$$S(v,T) = \frac{2hc^2v^3}{e^{\frac{chv}{kT}} - 1}$$
 (2.1)

Prior to detonation, the detector is collecting data from the scene within the field of view. This will be called the background signal and named S_{back} with a temperature T_{back} . This signal fills the entire field of view. Since the atmospheric temperature at detonation time is a known quantity, the form of the signal from the background is known for all frequencies. Calibration measurements were created using a blackbody that didn't completely fill the field of view. The field of view filled by the calibration blackbody relative to the entire field of view occupied by S_{back} changes the amplitude of the signal. A new variable, K, is introduced to represent this number. The other blackbody source of radiation is the detonation event. The signal from this source will be named S_{bomb} with a temperature T_{bomb} . The bomb occupies a dynamic fraction of the field of view during initiation, afterburn and decay. The fraction of the field of view occupied by the detonation will be represented by the new variable, F. The total signal in the field of view of the detector is then called S_{scene} . All terms are combined into Equation 2.2 to describe the signal from the scene at a given time step.

$$S_{Scene} = K[F \cdot S_{homb} + (1 - F) \cdot S_{bb}]$$

$$(2.2)$$

This is the basic form of the Equation that will be used to describe the detonation event recorded by the instrument. All quantities are known for each time step except

fractional field of view filled by the detonation and bomb temperature. These become the two variables found during the curve fitting process.

Fitting Procedures

Since Chapter III will provide a detailed review of the fitting procedures used, only an overview of the process will be discussed here. Fitting two variables simultaneously in an exponential Equation proved to be challenging. A modified method of bisection was created to fit the two variables. Event size was selected as the first variable evaluated. Root Mean Square Error (RMSE) was used as the convergence criteria. RMSE is described as the square root of the sum of residuals squared divided by the number of residuals. The calculation of RMSE for a single timestep is shown in Equation 2.18

$$RMSE = \sqrt{\sum_{i=1}^{nw} w_i (z_i - z_i)^2 / nw - 2}$$
 (2.18)

where i is the frequency location, w_i is the weighting of each data point, z_i is the data estimate using variables, z_i is the actual data being fit, and nw is the total number of data points used. The term nw-2 is the Degrees Of Freedom (DOF). For this research, weighting will be accomplished during PLEXUS data manipulation so w_i is 1 for all wavenumbers. Equation 2.18 is minimized during curve fitting using the bisection method described below.

The method of bisection fits an Equation by changing variables in decreasing intervals. The method uses a repeated halving of subintervals. The half with the smallest error is then identified. Equation 2.19 shows the interval magnitude for variable m at iteration n.

$$Interval_m^n = (0.5)^n \cdot \text{Varguess}_m \qquad (for \ n \ge 1)$$
 (2.19)

For each interval, the RMSE for *Varguess*, as well as the values of *Varguess* ± *interval* are found. The value with the lowest RMSE becomes the new *Varguess*. This method is repeated until an established criteria is met. Many methods in print use a maximum number of iterations as the exit criteria. To ensure the most accurate variable values, bisection was continued until three consecutive iterations with both variables yielded no change in RMSE. Other statistical values were computed as well. These values were computed to compare the fit of the FORTRAN code to the fit of the data using TableCurve. These values and their derivation are described in detail next chapter.

III. Approach

Introduction

Previous research provides a source of well-conditioned, calibrated data from explosive detonation tests. Through radiometric comparisons to data of the same event collected by other agencies, the validity of the data was verified. The approach taken in this research will be to use the existing data to find temporal profiles of event size and temperature for each event. Since data taken from the static detonations of Radiant Brass 3B are the most consistent, this data set is used.

Radiant Brass 3B consisted of 23 statically detonated events over the course of two nights. Three different explosive types and three different explosive amounts were used during this test. The ordnance was situated on solid ground and propped up on wooden tripods at a 45 degree elevation angle tail high. Each bomb face was pointed toward the instrumentation. The larger bombs were placed in clay craters tail high at the largest elevations possible

This chapter begins with a discussion of the data collection and calibration procedures used to create the data used in this research. A more detailed discussion on the collection and calibration of this data can be found in the BOMEM Users Manual, (2 and 3) or in Orson's thesis (17). This chapter will then explain the integration of the programs Mathematica, PLEXUS, FORTRAN and Table Curve used to process and interpret the data. The remainder of chapter will discuss the development and implementation of the numerical methods used to fit the data.

Calibration

During data collection, great care was taken to obtain the best data possible. Accurate calibration references were created using a calibrated black body with a known aperture setting. The blackbody was positioned a distance from the detector that simulated the size of the event in terms of fractional field of view. To avoid detector saturation, the anticipated fractional field of view seen by the detector at bomb initiation was used. From previous data, it was determined the size of a detonation event at 4750 m could be approximated by a 0.2" aperture at 76". The blackbody was set at it's maximum value of 1000°C. In this configuration, the MR-154 focused on the black body to determine the optimal gain settings. The detector gain settings were selected to produce maximum signal available without detector saturation. The final configuration settings were selected to maximize spectral range of the collected event signature with both detectors. The spectral range of the Mercury Cadmium Telluride (HgCdTe) detector was set at 500 to 6000 cm⁻¹. The spectral range of the Indium Antimonide (InSb) was set at 1800 to 6000 cm⁻¹. These spectral ranges cover most of the SWIR, the MWIR and LWIR regions. In this collection configuration both detectors have some overlap in spectral range for comparison between detectors. All event measurements were taken in zero scan mode utilizing only one sweep direction of the Michelson Interferometer. Finally, events were to be collected at 16 cm⁻¹ spectral resolution with temporal resolution of 0.047 seconds and at 4 cm⁻¹ spectral resolution and with resolution of 0.123 seconds.

Once gain settings, temporal resolution, spectral resolution and data collection times were set, calibration files were created. Calibration files were made with radiometric reference files. A calibrated blackbody source was used to build the

radiometric reference files at 700°C and 900°C. A Bomem Optics 74 milliradian collimator optics telescope was used during Radiant Brass 3B data collection. This telescope resulted in a roughly 360 m diameter field of view at the target point.

The Bomem MR Series FT-Spectroradiometer Design Overview and Theory section of the Bomem Users Manual (4) details the calibration and data collection process of the MR-154. The appropriate measurement equation for a blackbody source is shown as Equation 3.1. The units of $S_{meas}(v)$ is W/cm² str cm⁻¹ and will be called scene spectral radiance.

$$S_{meas}(v) = A_{opt}A_{bb} \frac{G_{elec}}{R^2} [L(v)Det(v)Tr_{opt}(v)Tr_{filter}(v)Tr_{atm}(v)]$$
(3.1)

where

 A_{opt} = area of instrument optical aperture

 A_{bb} = area of blackbody emitter

R = distance from calibration source to instrument

L(v) = blackbody spectral radiance W/cm² sr cm⁻¹

Det(v) = detector frequency dependent power responsivity

 $Tr_{opt}(v)$ = instrument optics wavelength dependent transmission

 $Tr_{filter}(v) = spectral filter transmission$

 $Tr_{atm}(v) = atmospheric transmission$

Gelec = electronic gain

The MR-154 has no filter so $Tr_{filter}(v)$ can be neglected. All system wavenumber dependant terms, Det(v) and $Tr_{opt}(v)$, as well as A_{opt} and G_{elec} can be grouped into one on term K(v). With these manipulations Equation 3.1 becomes Equation 3.2:

$$S_{meas}(v) = \frac{A_{bb}}{R^2} K(v) [L(v) Tr_{atm}(v)]$$
 (3.2)

Further assuming the transmission losses due to the atmosphere are negligible due to the short distance eliminates $Tr_{atm}(v)$. For a calibration sequence the A_{bb}/R^2 is constant

and can be combined into K(v). Lastly, when the event or calibration does not completely fill the system field of view, L(v) can be expanded to:

$$S_{Meas}(v) = K(v)[L_{hb}(v) + L_{hack}(v) + M^{Stray}(v)]$$
(3.3)

where

 $L_{bb}(v)$ = black body source radiance $L_{back}(v)$ = source background radiance $M^{Stray}(v)$ = system stray radiance term

To eliminate the source background, two measurements are taken at each calibration reference temperature, a source plus background and a background. These two reference measurements are subtracted to eliminate $L_{back}(v)$. Theoretically, this leaves only the contribution of the black body (bb) source in the S, L, and M quantities. Once $L_{back}(v)$ is subtracted, the equation becomes:

$$S_{bb}(v) = K(v)(L_{bb}(v) + M^{Stray}(v))$$
 (3.4)

A proper calibration procedure requires collection of a minimum of two reference temperatures, commonly called hot (H) and cold (C). These reference temperature files each need a separate background reference. The background reference theoretically removes all signal not associated with the calibration source. To create the background references, the blackbody radiation source is removed from the field of view. Any radiation in the field of view is captured and then subtracted from the hot and cold reference files. With these two background subtracted reference measurements, $M^{stray}(v)$ and K(v) are found by Equations 3.5 and 3.6.

$$K(v) = \frac{S_H(v) - S_C(v)}{L_H(v) - L_C(v)}$$
(3.5)

$$M^{Stray}(v) = \frac{L_H(v)S_C(v) - L_C(v)S_H(v)}{S_H^s(v) - S_C^{Meas}(v)}$$
(3.6)

Once $M^{stray}(v)$ and K(v) are determined, the equation to calibrate successive measurements is:

$$S^{Calibrated}(v) = S_{Meas}(v)K^{-1}(v) - M^{Stray}(v)$$
(3.7)

Equation 3.7 is essentially a mathematic correction applied to a 'sensed' unknown signal. This assumption used during calibration is only valid if all operating parameters of the system remain constant between reference point acquisition and the unknown measurement. Since the MR-154 collects data on both sweep directions of the interferometer, two sets of calibration constants are created.

Linearity is a big assumption in Equation 3.7. This assumption requires linearity in the system and detector. For the large radiance and spectral range required to measure a detonation event, linearity in the InSb detector is a valid assumption. For the HgCdTe detector a quadric calibration is more appropriate. The details of a quadratic calibration can be found in the Bomem users manual (5, 3:109-111).

Data Collection

The collection of data of an unknown event is considered in much the same way as the radiometric reference was taken during calibration. The unknown event is recorded using the same gain, resolution and detector settings used during calibration. All of the assumptions that were made between Equation 3.1 and Equation 3.2 are still valid. However, the measurement of a dynamic unknown blackbody source at a great distance changes the Equation beyond the form shown in Equation 3.2. Equation 3.2 is recalled as Equation 3.8.

$$S_{meas}(v) = \frac{A_{bb}}{R^2} K(v) [L(v) Tr_{atm}(v)]$$
 (3.8)

For measurement of an unknown signal, all of the radiation the detector is receiving come from within the field of view. The detector signal received will become scene spectral radiance represented by the term $S_{scene}(v)$. The term $Tr_{atm}(v)$ becomes very important as distances increase and can not be discarded as it was during calibration. Chapter II discussed the effects of atmospheric absorption across an IR region of the spectrum. This term remains in the Equation. The atmospheric absorption will be removed as much as possible using PLEXUS. The term A_{bb}/R^2 remains constant as the portion of the field of view considered in the radiometric reference files. This quantity can be defined as the solid angle between the detector and the blackbody aperture size. This number can be calculated and will be used later. For now, it's considered a constant and is included in K(v). L(v) is expanded into the radiation sources expected within the FIELD OF VIEW of the detector. For a detonation event, these terms are radiation from the explosion, $S_{bomb}(v)$, and radiation from everything else in the FOV, $S_{back}(v)$. Prior to bomb initiation, the portion of the field of view filled by detonation signal is zero. After detonation the fraction becomes a number that changes with time as the event goes through the phases of initiation, afterburn and decay. To account for the dynamic portion of the field of view filled by the detonation event, a new variable F is introduced. F represents the relative fraction of the field of view occupied by the explosion. The rest of the field of view is then represented by (1-F). The new form of the function now becomes Equation 3.9.

$$S_{\text{scene}}(v) = \text{Tr}_{\text{atm}}(v) \cdot K(v) [F \cdot S_{\text{homb}}(v) + (1 - F) \cdot S_{\text{hack}}(v)]$$
(3.9)

This Equation represents the signal received by the detector. This total is the sum of the bomb radiation and background black body radiation. The term $S_{scene}(\sigma)$ represents the calibrated spectral scene radiance data created by the instrument Aquire software. To extract detonation temperature and size at each time step, the wavenumber dependant Planck distribution introduced as Equation 1.5 is recalled as Equation 3.10. Equation 3.10 describes the intensity and form of spectral radiance from a gray body as a function of wavenumber and temperature.

$$S(v,T) = \varepsilon(v) \frac{2hc^2v^3}{e^{chv}/kT}$$
(3.10)

The terms $S_{back}(v)$ and $S_{bomb}(v)$ in Equation 3.9 are replaced with their respective blackbody forms of Equation 3.10 Gray body effects are placed in the term K(v) removing the $\varepsilon(v)$ term from Equation 3.10 The temperature used in $S_{back}(v)$ is represented by T_{back} and will be the ambient atmospheric temperature at data collection time. The temperature in $S_{bomb}(v)$ is given the name T_{bomb} and is one of the two numbers to be found.

Finally, an atmospheric transmittance profile is created using PLEXUS. The transmittance profile uses the atmospheric temperature, atmospheric pressure, humidity and distance to detonation event to create a file representing atmospheric transmittance at each wavenumber location. If the transmittance value was below 0.4, this division produced excessive scene spectral radiance values. All wavenumber locations with a transmittance value of 0.4 or less were considered less accurate than other frequencies and scene spectral radiance was set to zero for that frequency. New scene spectral radiance values were created at wavenumber locations having transmittance values greater than 0.4 by dividing by the transmittance value. The PLEXUS corrected data is

identified by the * superscript. The form representing transmittance corrected spectral scene radiance at one time step becomes Equation 3.11:

$$S(v)_{scene}^* = K(v) \cdot F\left\{\frac{2hc^2v^3}{Exp(chv/kT_{bomb}) - 1}\right\} + K(v) \cdot (1 - F)\left\{\frac{2hc^2v^3}{Exp(chv/kT_{back}) - 1}\right\}$$
(3.11)

The asterisk on $S(v)_{scene}^*$ indicates the original data has been PLEXUS corrected. This equation represents the data for each time step evaluated over all frequencies. The calibration term K(v) is distributed so that each term may be discussed independently.

Consider the first term of Equation 3.11. This term represents the radiation received by the detector due to the detonation event. Prior to detonation, F equals zero and the only radiation source in the field of view is the background. At any time after bomb initiation, F represents the fractional field of view of the event at that time step. This value is relative to the portion of the field of view filled by the black body references during calibration. By relating the value of F to the known fraction of the field of view filled by the reference blackbody, event size can be determined

When the temperature of the event falls between or near the hot and cold radiometric reference files, the value of K is well described. Recall for all calibrations during RB3B, hot and cold references were created at 1173 and 973 Kelvin respectively.

The second term in Equation 3.11 describes the scene radiance values created by the Acquire software due to background radiation. Before detonation, F equals zero and all radiation received is due to the background scene for that time step. Recall that K is a linear calibration parameter created by recording radiation from known sources and subtracting background radiation. Therefore, a perfect calibration over all temperatures would yield a zero value for all frequencies when there is no signal other than

background. However, calibrated scene radiance values observed are not zero. For radiation due to background, K may not be an appropriate value since the ambient temperature of around 300 Kelvin is not between or even near the hot and cold radiometric reference temperatures of 1173 and 973 Kelvin. In order to correct the spectral scene radiance values for all data, average values of the background prior to bomb initiation are computed. Since the signal from the event is two-three orders of magnitude smaller than the signal of the background, this can be done without adversely affecting detonation data. The background average values are subtracted from the PLEXUS adjusted data to create a new data set representing scene radiance. With this correction, the radiation at the detector is described by the new Equation 3.12.

$$S(v, F, T_{bomb})_{scene}^{**} = F \left\{ \frac{2hc^2v^3}{Exp(chv/kT_{bomb}) - 1} \right\}$$
(3.12)

The term $S(v, F, T_{bomb})_{scene}^{**}$ has two asterisks representing the two corrections made to the data, PLEXUS transmittance correction and background signal subtraction. For a given time step, the equation has only two variables when considered over all frequencies. This is the final form of the function used to find bomb temperature and detonation size at each time step.

Data Interpretation

Once corrections were made to the data removing atmospheric absorption and background signal, the corrected data was used to describe a detonation event. The two variables in Equation 3.12 are bomb temperature and fractional field of view. The data was fit using a simple least-squares minimization procedure. Curve fitting two variable in a non-linear equation using least squares can be accomplished a number of ways. The

method chosen in this work was bisection for two variables consecutively. Non-linear fitting is an iterative procedure that begins with an initial set of estimates of the variables. Regardless of the method used to converge to the minimum least-squares solution, a point-by-point sum of squared residuals must be calculated for each iteration. Recall that the data correction method described previously included subtraction of the average background signal from all time steps. Therefore, any time step with no event in the field of view essentially contained no data. Curve fitting procedures were not applied to the data for time steps prior to detonation. At bomb initiation, an initial estimate for bomb temperature of 1500 Kelvin was used. The initial estimate for relative fractional field of view was set as the unitless factor 2. Each iteration of the curve-fitting procedure would then calculate the least-square error for the function using the initial values stated above. The form of the least-square error used for convergence is the Root Mean Square Error (RMSE). The form of the RMSE is shown in Equation 3.13.

$$RMSE = \sqrt{\frac{\sum_{j=1}^{nw} \left(s_{j}^{**} - s_{j}^{F, T_{bomb}}\right)^{2}}{\left(nw - 2\right)}}$$
(3.13)

where j represents the frequency location of the corrected data. The number of frequency locations containing data is nw. s_j^{**} represents the value of the corrected data at each frequency. The denominator (nw-2) represents the Degrees of Freedom (DOF). This quantity is defined as number of variables being fit subtracted from number of data points used.

New estimates of each parameter were tested at each iteration. The new estimates were created and applied using the bisection method. The original estimate was adjusted in decreasing intervals described by Equation 3.14.

$$Estimate_{New}^{X} = Estimate_{Old}^{X} \pm (0.5^{i}) \cdot Estimate_{Original}^{X}$$
(3.14)

where X represents the variable being estimated and i is the iteration step. The values above and below the initial estimate were evaluated at each iteration. The RMSE for the original estimate. The estimate above and the estimate below were calculated. Due to the form of the data, F was the first variable fit at each iteration. The estimated value of T_{bomb} was used with the three estimates of F. The F estimate resulting in the minimum RMSE was then taken as the new value to be used through the next iteration. The established value of F was then taken with the three estimates of bomb temperature within the same iteration step. The value of T_{bomb} resulting in the lowest RMSE became the value used in the next iteration. In successive iterations, the interval of the variable change is halved until an established criteria is met. The criteria used for this research was to stop iterating when the value of the step size fell below the computer resolution.

When fitting two variables, the process of adjusting one of the variables affects the best-fit value of the other variable. To ensure best fit values were as accurate as possible, the iteration process was repeated. The new iteration set was started using the variable values established in the previous iteration set. This process was repeated until the RMSE for the final estimated values remained the same over two consecutive iteration sets. The program Table Curve was used to verify the values of the two variables. The values found by TableCurve were within 1-2 percent of the values found with the bisection method explained above. Details of the TableCurve comparison can be found in Chapters IV and V.

IV. Procedures

Introduction

Chapters I. II and III discussed the theory and development of the concepts and tools used during this research. This chapter describes the specific details of the process as it was developed. First, an explanation of the format of the ASCII data files containing event calibrated scene spectral radiance will be discussed. This will lead to a discussion on how to determine dimensions of the ASCII data and import the data into the FORTRAN program. Chapter IV continues with the creation of PLEXUS transmittance files based on the form of the data and the atmospheric conditions at data collection time. Next is a discussion of how the PLEXUS transmittance profile is used to remove atmospheric signal loss from the data. The discussion continues with an explanation of how the average background signal was determined and subtracted from the data. The process used to fit this final form of the adjusted data and the statistical quantities generated is discussed next. The discussion continues with a description of the data files created and their format. Finally, how TableCurve was used to verify curve fit results and Mathematica was linked to the FORTRAN program for graphical interpretation of the new data will be discussed.

Data Manipulation

The initial approach taken in this effort was to use Mathematica as the data manipulation and calculation program. Mathematica provides a combination of computational and graphical tools. However, the format and dimensions of the data files didn't work efficiently in the Mathematica environment. In order to ingest ASCII data,

Mathematica requires the dimensions (number of rows and columns) as an input. However, the data files had different dimensions depending on sensor used, spectral resolution selected and number of measurements taken during a data collection sequence. In order to process data files without calculating dimensions first, FORTRAN was selected as the program to be used for data manipulation and iterative calculations. The final version of the FORTRAN code is included as Appendix 1.

The process of creating a FORTRAN program began with the following objectives. First the program should be able to read the data regardless of dimensions. Second, the program needed to be able to place the data into arrays to be used during calculations. Third, the code had to be able to combine different types of data since the input data did not always have the same dimensions. Fourth, the program had to accept and use different parameters. Finally, the program had to create new data files containing the results of the calculations.

The inputs to the program would be the locations of the raw data created in previous research, the location of the PLEXUS transmittance profile, the names and locations of the data files created by the program and all user variables used in the calculations. The final version of the FORTRAN program performed all functions as directed.

All of the Input/Output (IO) information was placed in a file named "infile.txt". The IO file could be changed by editing the file directly or by running a Mathematica script built to edit the IO file. The Mathematica code used to create the IO file and provide graphical data plots is included as Appendix 2.

The files containing the detonation event data were identified and organized. One ASCII data file represents the total calculated scene spectral radiance at all time steps recorded. Each data file is organized in rows representing the intensity value at a given frequency for all time steps. Columns represent the value at a given time step for all frequencies. Table 4.1 shows the format of a sample ASCII data file.

Table 4.1 ASCII Data format of Detonation Event

Frequency (cm^-1)	$t_{n=1}$	$t_{n=2}$	t_n	$t_{n=nt-1}$	$t_{n=nt}$
499.527	Data _{1,1}	Data _{1,2}	Data _{1,n}	Data _{1,nt-1}	Data _{1,nt}
501.455	$Data_{2,1}$	Data _{2,2}	$Data_{2,n}$	$Data_{2,nt-1}$	Data _{2,nt}
503.3839	Data _{3,1}	Data _{3,2}	Data _{3,n}	Data _{3,nt-1}	Data _{3,nt}
$freq_m$	Data _{m,1}	Data _{m,2}	$Data_{m,n}$	Data _{m,nt-1}	Data _{m,nt}
5998.1771	$Data_{nw\text{-}1,1}$	$Data_{nw\text{-}1,2}$	$Data_{nw\text{-}1,2}$	$Data_{nw\text{-}1,nt\text{-}1}$	$Data_{nw\text{-}1,nt}$
6000.1058	$\mathrm{Data}_{\mathrm{nw},1}$	$\mathrm{Data}_{\mathrm{nw},2}$	$Data_{nw,3}$	$Data_{nw,nt\text{-}1}$	$Data_{nw,nt}$

where nw represents the number of frequency divisions and nt is the number if time steps in each data set. The first column represents the frequency for each row (in wavenumbers). The remaining columns held data values at different time steps. Since there is a column for frequency values the total number of columns in the raw data is nt+1 and the dimensions of the data is nw by nt+1.

It is important to recognize that the frequency values are spaced at equal intervals but are not integer values. This is considered when applying the PLEXUS created data.

PLEXUS data is created with frequency intervals at integer values.

Once the program read the data, the information could then be processed in a logical order. The data was generally processed column by column. This order represents an interrogation of all frequencies simultaneously as time progressed.

PLEXUS Application

The PLEXUS/MODTRAN program was discussed in Chapters I and II. The program creates a transmittance profile representing atmospheric absorption or scattering signal loss. Frequency intervals are determined by the user of the software. However, the frequency values can only be defined in integer intervals. In order for a row-by-row calculation of the radiance data with the transmittance data, the intervals and number of rows had to match. Therefore, a new transmittance profile was created for each data set. The new profile was built by interpolating the value of the transmittance from the closest two values surrounding each raw data frequency location. The interpolation was done using linear interpolation based on divided differences. The assumption of a constant slope is made over the interval (x_1, x_2) with the corresponding values y_1 and y_2 . A value for y_i can be found at a given value x_i . This is true assuming a constant slope within the interval. With a constant slope, the divided difference over the interval (x_1, x_2) is the same as the divided difference over the interval (x_1, x_2) as shown in Equation 4.1

$$\frac{(y_i - y_1)}{(x_i - x_1)} = \frac{(y_2 - y_1)}{(x_2 - x_1)} \tag{4.1}$$

Solving for y_i yields Equation 4.2

$$y_i = \frac{(y_2 - y_1)(x_i - x_1)}{(x_2 - x_1)} + y_1 \tag{4.2}$$

To minimize interpolation error, PLEXUS transmittance files are created with frequency resolution of the integer number closest to the frequency resolution of the data

being corrected. After a transmittance profile is created in array form, the original data can be divided by the transmittance value at each frequency. If the transmittance profile exactly predicted the amount of signal lost to the atmosphere at each frequency, the result would be an exact representation of the signal from the source. However, the prediction is not exact and errors in the process appear in the corrected data. These errors are greatest where values of transmittance are low. Figures 4.1 through 4.4 show the raw data and PLEXUS corrected data for both sensors at a time step immediately after bomb initiation.

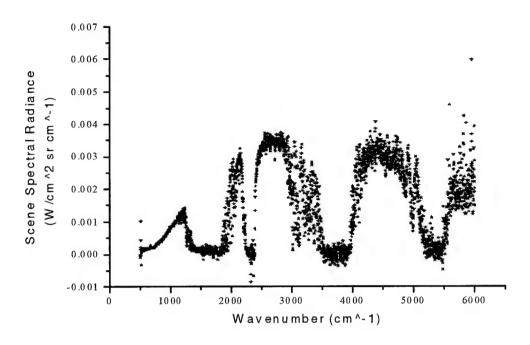


Figure 4.1 HgCdTe Raw Data

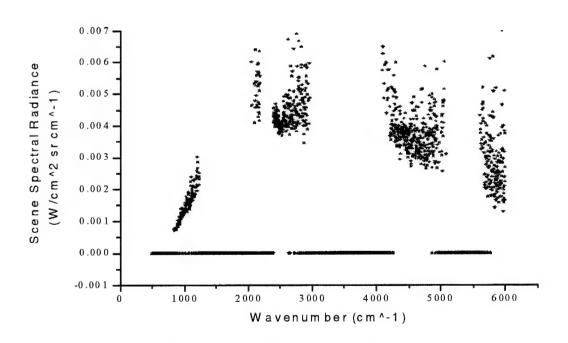


Figure 4.2 HgCdTe Corrected Data

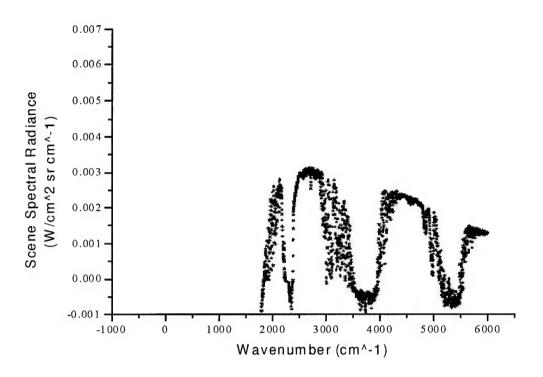


Figure 4.3 InSb Raw Data

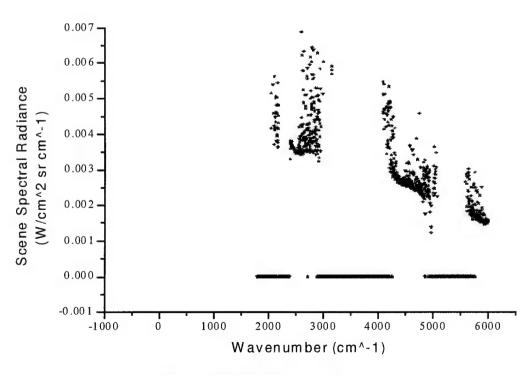


Figure 4.4 InSb Corrected Data

Figures 4.1 through 4.4 also show the frequency range of each sensor. The HgCdTe sensor produced a profile with more noise but had a greater frequency range. The InSb sensor produced data with much less noise but the frequency range did not extend into the Long Wave InfraRed (LWIR) region of the spectrum. These sensor characteristics are important to remember to ensure the best data set is created during the PLEXUS adjustment.

Background Signal Subtraction

The final correction made to the data was to remove the average background signal prior to detonation from the data set. The explanation of the background signal subtraction is detailed in Chapter III. Without subtracting the average signal profile due to background radiation, the curve-fitting process would fit to an Equation including two Planck functions instead of one. Additionally, subtracting the average background profile eliminates the need to find the calibration constant, K, to be used in the two Planckian version shown in Equation 3.5.

The average background profile was built by summing the pre-detonation PLEXUS corrected data profiles over a number of time steps. The number of time steps used was then divided into these totals. Although the first two time steps of the data appeared to be representative of the background signal, the third through twenty-seventh time steps were used to avoid any background average contamination due to collection process initiation. Figures 4.5 and 4.6 show typical average background signal profiles for each detector.

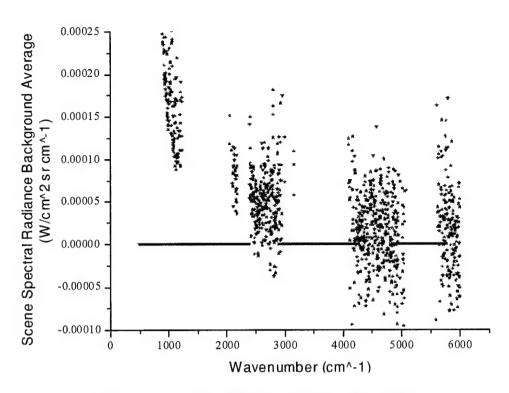


Figure 4.5 Average HgCdTe Background Signal

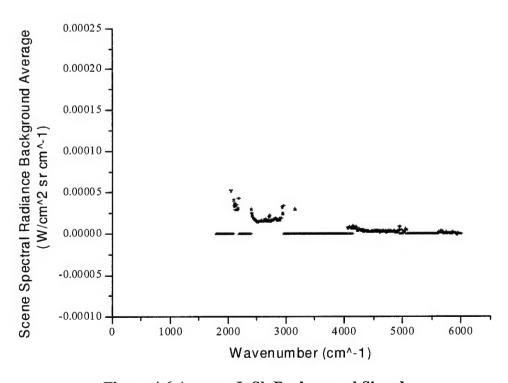


Figure 4.6 Average InSb Background Signal

With the average background profile subtracted from the data, the only data remaining in each time step prior to event initiation is noise. No information could be inferred from the pre-detonation data. However, the conditions filling the field of view are known quantities. The field of view is observing the background which is basically at the ambient atmospheric temperature. The variable F representing the relative fractional field of view filled by the event is zero prior to detonation. To avoid processing the data during the curve-fitting process, a threshold 'trigger' was built into the program which determined when the data at each time step would be processed. The method selected was to find the average pre-background subtracted intensity within the frequency range of 2400-2800 wavenumbers. This interval was selected for three reasons. First, the interval is included in the range of both sensors. The second reason this region was selected was the PLEXUS values were generally greater than 0.4. The final reason for selecting this interval was the largest increase in intensity was expected in this region for the temperatures of the events expected. The average background signal within this region was easily found since averages of the entire data range were calculated during background average calculation. This average value was then compared to the average within the same interval of the actual data at each time iteration.

If this average was larger than the actual data, the time step was given values of scene temperature equals 300 Kelvin and relative fractional field of view due to event, F, equals zero. The first time the average value fell below the corrected data average, event initiation is assumed and the curve fitting process begins for that time step. The values of 1500 Kelvin for temperature and 2.0 for F were used as initial estimated for the first time step processed. In successive time steps, the values determined during the fitting process

of the prior time step were used as initial estimates. Once both corrections were applied to the data, the program started process of fitting the corrected data to the function.

Curve Fitting

A subroutine was built within the program to test the estimates being made during the bisection process described in Chapter III. The subroutine created statistical values representing how well the function matched the actual data using the estimates provided. These values were used during the bisection method to converge to the best values of T_{bomb} and F. The form of these statistical values are shown in Equations 4.3 through 4.9.

Sum of Squares due to Error:
$$SSE = \sum_{j=1}^{nw} \left(S_j^{**} - S_j^{F, T_{bomb}} \right)^2$$
 (4.3)

(Sum of Residuals Squared)

Sum of Squares about Mean:
$$SSM = \sum_{j=1}^{mv} \left(S_j^{**} - \bar{S} \right)^2$$
 (4.4)

Coefficient of Determination:
$$r^2 = 1 - \frac{SSE}{SSM}$$
 (4.5)

Degrees of Freedom
$$DOF = n - m$$
 (4.6)

Mean Square Error
$$MSE = \frac{SSE}{DOF}$$
 (4.7)

Fit Standard Error (Se)
$$RMSE = \sqrt{MSE}$$
 (4.8)

F-statistic
$$F = \frac{MSR}{MSE}$$
 (4.9)

 S_j^{**} represents the corrected data at each frequency. $S_j^{F,T_{bomb}}$ is the value at each frequency given by the function using the estimates of T_{bomb} and F. \bar{S} is the mean value over all frequencies in the time step. The total number of data points used is n and m is the number of variables in the function being fit. The exact form of these statistics was taken

from the TableCurve 3-D Users Manual (23,E-5). The form was duplicated since TableCurve was used to verify fit results derived by the program and show graphical output.

Data Created

An execution of the program would create eight files in ASCII format. The first output file created by the program was a PLEXUS transmittance profile with interpolated frequency values matching the frequencies of the event data file. The next two files were created by solving for temperature using Planck's Equation. These files were created to investigate the composition of the main data file. The second file created was a temperature as a function of frequency and raw intensity at a selected time step. The third data file built was a temperature file for all times and frequencies. The fourth output data file contained all the statistical fit values described above for each time step processed. The fifth ASCII file contained the profile of the average background signal prior to detonation. The sixth file held the average value of the 2400 through 2800 wave number frequency interval. The seventh file was the event temperature found by the curve fitting process as a function of time. The eighth output file contained the value of the variable *F* at each time step determined by the fit. The final data file created during program execution was the final value of RMSE describing the fit as a function of time.

Interpretation of New Data

Reducing the original data was accomplished by a FORTRAN program created as part of this research. The FORTRAN program could be initiated by a Mathematica script which provided the IO details. Data generated through execution of the program was

TableCurve 2-D Version 5.0. TableCurve was used to check the fit of the derived variables to the data using the formula derived in Chapter III. TableCurve also proved valuable in providing a graphical representation of Planckian curve overlaying the data population. The second program used to interpret the derived data was Microcal Origin Version 6.0. Microcal Origin organizes data in spreadsheet format. The spreadsheet format proved useful in displaying three-dimensional graphs used to compare data.

V. Results

Introduction

This chapter details the results of the data processing and analysis accomplished during this research effort. The results indicate event characterization may be possible after data reduction. Furthermore, the large data files containing the event could be quickly reduced with a few manipulations. The original ASCII data files were between 3-10 Mega-Bytes each. Each file was reduced with the program described in previous chapters into three manageable 20 Kilo-Byte files containing the temporal description of relative fractional field of view, *F*, bomb temperature and fit error. Due to the large amounts of data, only a portion of the events and data will be described in this chapter and in the following appendices. For continuity, the events covered in this work are the same as the events investigated in previous research.

Discussion will start with a general overview of the three dimensions of the initial data. This is followed with a discussion of the data processing as it was done step-by step. This discussion includes the processes used to verify each step. Undesirable effects on the data from the processing are described. Finally, qualitative examination of the graybody characteristics and the features versus time curves are discussed.

Data Overview

The creation of data manipulation and calculation tools was a success. The programs created reduce large data files consisting of abstract quantities of wavenumber and scene spectral radiance representing the IR signal of an event. The large data sets are

converted to understandable data representing the temporal behavior of the event. The initial form of the data is shown in Figure 5.1.

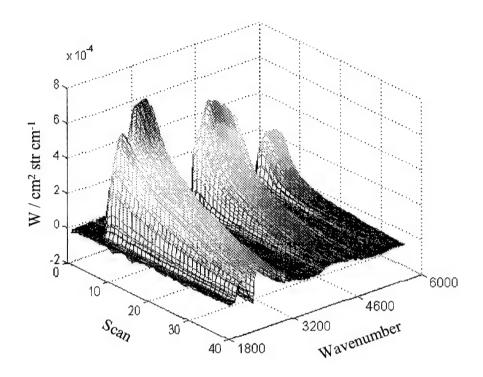


Figure 5.1 Three-Dimensional View of a Typical Event. (17)

This event was collected at 16 cm⁻¹ spectral resolution using the InSb detector.

Each wavenumber bin is roughly 8 cm⁻¹ apart. Each scan represents a 0.047 second time step. This figure represents only 1.88 seconds of event data. The entire data file included 27 seconds of data. Vertical axis is calibrated scene spectral radiance as calculated by the MR-154 and *Acquire* software. Atmospheric absorption causes the zero values located between intensity peaks.

A single slice of the Figure above displays the spectral profile at a single time step measurement. Figure 5.2 shows the spectral profile of a time step immediately after detonation.

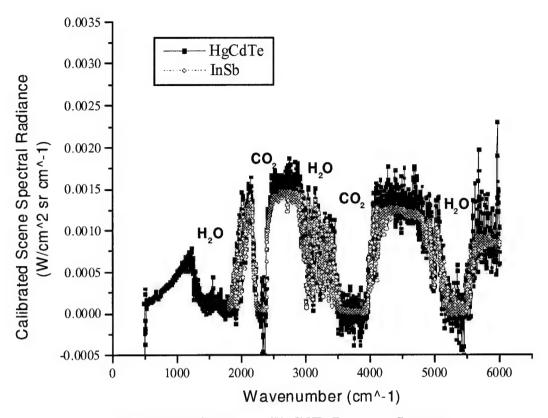


Figure 5.2 InSb Versus HgCdTe Detector Spectra

The spectral resolution for the figure is 4 cm⁻¹. The interval of the frequency steps for both detectors is 1.929 cm⁻¹. The spectra collected with the InSb detector is represented by the darker line ranging from 1800 to 6000 cm⁻¹. The HgCdTe spectra is the more noisy data ranging from 500 to 6000 cm⁻¹. Atmospheric absorption bands degrade or eliminate the signal in several frequency intervals. The primary atmospheric absorption molecules in these intervals are superimposed on the FIGURE.

The noise levels in the HgCdTe detector increase with increasing wavenumber. The maximum noise range for the HgCdTe is +/- 0.0001 W/(cm² str cm⁻¹). The corresponding noise range for the InSb detector is approximately +/- 0.00002 W/(cm² str cm⁻¹). Spectra collected with the InSb detector contained less noise; therefore, the data most often analyzed was collected with the InSb detector.

The events processed include data collected at two different spectral resolutions, 4 cm⁻¹ and 16 cm⁻¹. The specific spectral features of the events are not investigated in this research. The work done here eliminates the spectral information of the data and infers the temporal behavior of the event's size temperature and graybody fit error. However, the spectral resolution possibly influenced the results of the data processing sequence. This possibility is discussed later. During data processing, the program could be instructed to include instantaneous profiles of the data at a given time step. This capability was included in the program so further research of data created by the MR-154 could be investigated through its temporal or spectral characteristics. The specific data manipulations applied to the data can be explained using this feature. This will be done by following the data shown in Figure 5.2 through each step of the program as it executes.

After the event data file is identified, a transmittance profile must be created using the atmospheric conditions during data collection as PLEXUS input. The resolution of the created transmittance file should be at the closest integer value to the spectral resolution. For this data at 1.929 cm⁻¹, a transmittance file is created at 2 cm⁻¹ intervals. The first data manipulation is to interpolate the transmittance values to values at frequency steps in the data file. Once this is accomplished, the transmittance values are divided into the original data. Frequency locations with transmittance values lower than a cutoff value provided by the user are set to zero. The resultant data after this manipulation is shown in Figure 5.3

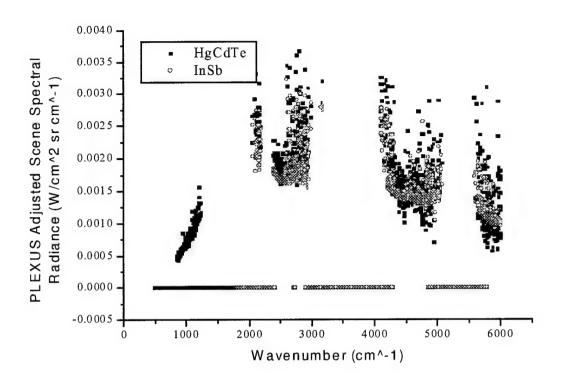


Figure 5.3 PLEXUS Adjusted Scene Spectral Radiance

Figure 5.3 shows the results of atmospheric adjustment. Division by cutoff values too large causes a loss of data, cutoff values too low result in overestimated values. The value of 0.4 was used in all transmittance corrections. The average values at each frequency prior to detonation are then calculated to build a background scene spectral radiance profile. This average pre-detonation signal is subtracted as described in Chapter IV to correct the calibration near ambient temperatures. The average background profile subtracted from the post detonation data were shown in Figures 4.5 and 4.6. Since the magnitudes of the average background profiles were orders of magnitude smaller than the detonation data, the final form of the data is effectively unchanged.

The final manipulation of the adjusted data is curve fitting. The form of the function to describe the event as derived in Equation 3.6. This Equation is recalled as Equation 5.1.

$$S(v, F, T_{bomb})_{scene}^{**} = F \left\{ \frac{2hc^2v^3}{exp(chv/kT_{bomb}) - 1} \right\}$$
 (5.1)

The corrected data is fit to this Equation as described in Chapter IV. At the end of each time iteration, the final values of F, T_{bomb} and the RMSE are recorded. These parameters were compared to the values computed by TableCurve. Figures 5.4 and 5.5 show the final form of the data and the best-fit curve found by TableCurve for the InSb and HgCdTe sensors respectively.

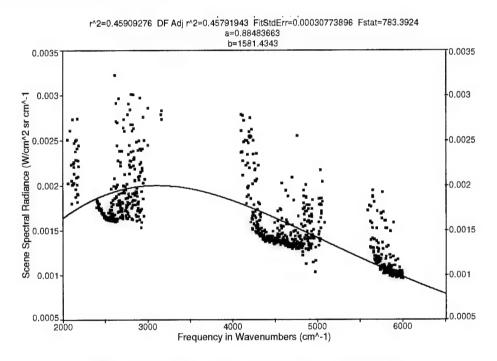


Figure 5.4 InSb TableCurve Data Verification

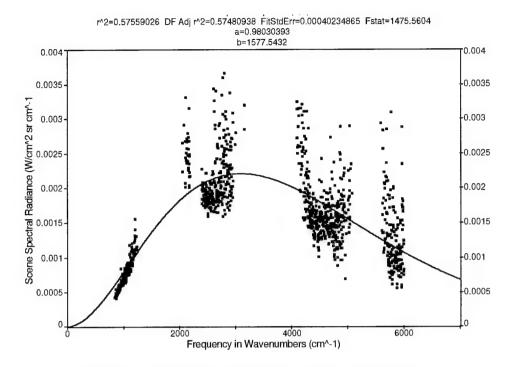


Figure 5.5 HgCdTe TableCurve Data Verification

Notice the offset of the curve from the heavily populated data sections. This effect was considered when selecting a cutoff for the transmittance value. When a lower value was used, much of the data in the 750 to 1250 wavenumber region was lost. This would sometimes cause erroneous curve fitting during the decay phase of the event evolution. Chapter VI includes a discussion on possible corrections to this problem as part of further research.

During program execution, a file was created containing the final values of the variables and the statistical quantities describing the quality of the fit of these variables. As a comparison, the values of the time step followed above are compared using values from this file. Table 5.1 shows the values of the fit variables and RMSE determined by the program compared to the same values from TableCurve.

Table 5.1 Variable Fit Comparison

	InSb F	$\begin{array}{c} \textbf{InSb} \\ \textbf{T}_{\textbf{bomb}} \end{array}$	InSb RMSE	HgCdTe F	HgCdTe T _{bomb}	HgCdTe RMSE
FORTRAN	0.89847	1575.070	3.0780e-4	0.97714	1578.887	4.0235e-4
TableCurve	0.88484	1581.434	3.0774e-4	0.98030	1577.543	4.0235e-4

Overall, the values calculated by the FORTRAN program were very close to the values derived by TableCurve. A statistical analysis of an entire data file was performed to test the program through a detonation sequence. The data files used included the time step evolution described above.

As part of its fitting procedures, TableCurve calculates values above and below each variable representing the 95% confidence interval for each variable. In most cases, the FORTRAN program calculated values within the 95% confidence intervals. The only time the values strayed from the TableCurve intervals was with the InSb during the decay phase of an event. This is believed to be due to the lack of data below 1800 wavenumbers. Without the low wavenumber reference, the data is missing a reference for half of the Planckian curve. The 95% confidence intervals calculated are included in Figures 5.6 through 5.9 showing the InSb and HgCdTe fit comparison of variables for a Radiant Brass 3B Event number 3.

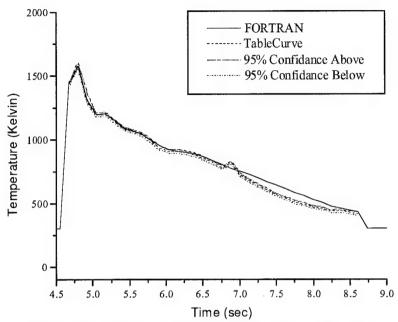


Figure 5.6 Event 3 InSb Temperature Comparison

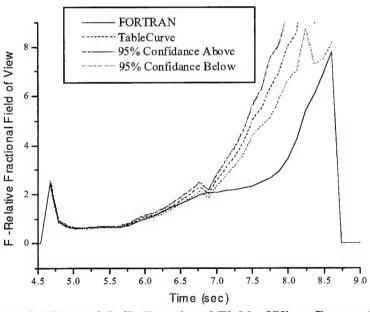


Figure 5.7 Event 3 InSb Fractional Field of View Comparison

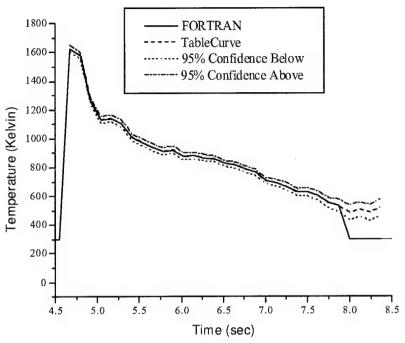


Figure 5.8 Event 3 HgCdTe Temperature Comparison

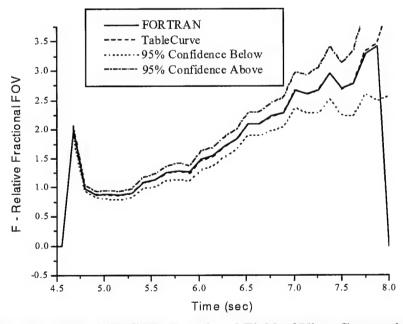


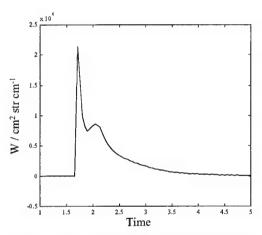
Figure 5.9 Event 3 HgCdTe Fractional Field of View Comparison

The deviation from the TableCurve values shown in Figure 5.7 is probably caused by the frequency range limitations of the InSb as discussed above. The deviation of our values of F from the TableCurve values occurs as the intensity of the collected signal is

decreasing rapidly during event decay. Figures 5.8 and 5.9 show that the noise on the HgCdTe detector causes the confidence interval to be wider. However, the FORTRAN code generated values fit the TableCurve values for all data from the HgCdTe detector.

Event Classification

During his work, Orson integrated the intensity value at all frequencies for each time step (17). In this manner, an energy versus time profile is created. He estimated this profile described the event as a decaying gray body. The results of this method indicated two different time evolution patterns. The two time modes were identified to classify different types of explosives. Figures 5.10 and 5.11 from his thesis show these two modes:



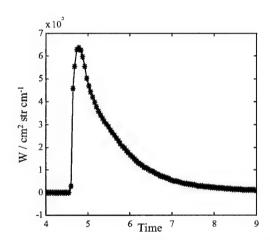


Figure 5.10 Evolution Mode One (17)

Figure 5.11 Evolution Mode Two (17)

Figure 5.4 shows the first time evolution mode. This mode was the expected time decay mode and has two well-defined peaks. This pattern described the phases of initiation, afterburn and decay. The second time evolution mode showed an initiation followed by a growth period resulting in the afterburn peak becoming the largest apparent radiance value. The decay rate of this mode was normally slower than mode one.

The data produced from this work shows the two modes also can be used to describe the temporal evolution of the event Temperature. Using data from events of the same explosion species produced the same time mode profile when data collection conditions were similar. Some collection events showed inconclusive results due to variability in look angle, impact surface and impact vector. Data adversely affected by these factors generally displayed the same temporal profile during the first two seconds following detonation. The convention of identifying events as explosive types A and B is consistent with prior research in this area. Two species in particular could be described by different time modes.

The first event species investigated here is the large type B explosive. Large type B detonations were clearly identifiable by distinct afterburn feature in the temperature profile at approximately 0.5 seconds after bomb initiation. Figures 5.12 through 5.14 show the temporal profiles of two large B events, collected at different spectral resolutions.

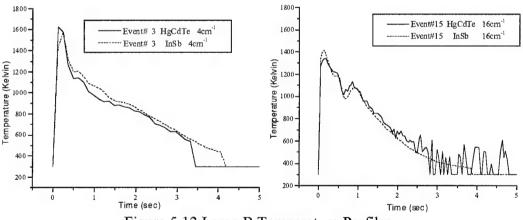


Figure 5.12 Large B Temperature Profiles

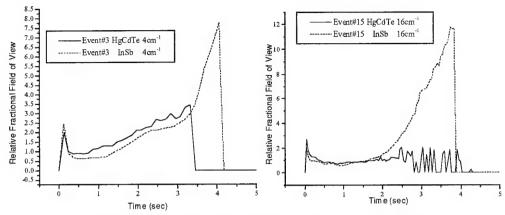
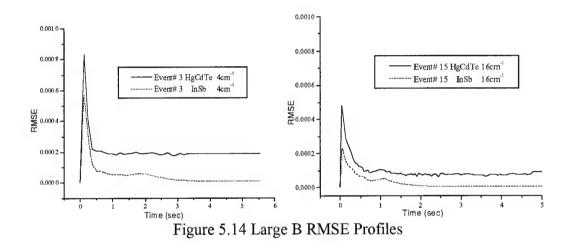


Figure 5.13 Large B Fractional Field of View Profiles



Data collected on large B events consistently displayed the afterburn feature from 0.75 to 1.00 seconds in the temperature profile. The afterburn is followed by a steady decay out to 5 seconds. The expected slow rise of the variable F is observed clearly in higher frequency resolution data.

The second type of data investigated was collected on small events using type A explosives. This event represents the largest number of data sets in ASCII format. Figures 5.15 through 5.17 show the temporal profiles of small A events.

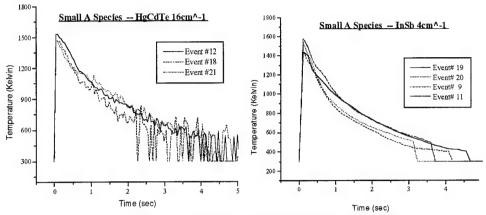


Figure 5.15 Small A Temperature Profiles

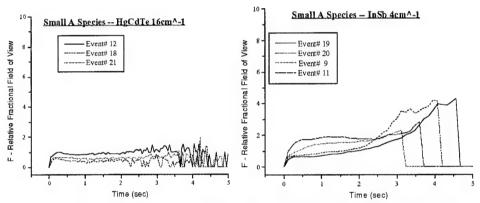


Figure 5.16 Small A Fractional FIELD OF VIEW Profiles

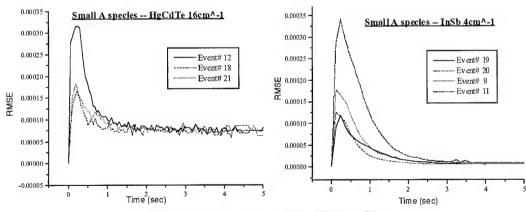


Figure 5.17 Small A RMSE Profiles

The temperature profile of small type A events matched time evolution mode two.

A small afterburn feature can be distinguished on some temperature profiles. Generally,

small A detonations displayed an instantaneous initiation followed by rapid decay beginning almost immediately. The decay rate decreased toward the end of the event sequence. It may be possible to fit these temporal profiles to an exponential decay model. The fractional field of view versus time profiles were highly variable. The general pattern seemed to be a smaller and nearly constant size throughout the first half of the event sequence. During the second half of the event sequence, about 2 seconds after detonation, the size of the event indicates a gradual growth event size.

Data from other species was analyzed as well. Graphical representations of these species were consistent with explosive type. Small A explosives displayed the same time evolution features as large A and medium A detonations. Similarly, large B explosives displayed the same time evolution features as small B and medium B detonations.

The FORTRAN and Mathematica programs created should be able to read and interpret any BOMEM MR-154 generated ASCII data set with little or no modification. Future research in this area should be much easier with the programs created during this thesis.

VI. Conclusions

Introduction

This chapter addresses the conclusions reached through the process of manipulating data collected during previous research. The source of the data investigated was the calibrated detonation event data collected using the Bomem MR-154 FTIR to capture detonation signatures during the Radiant Brass tests at Fallon NAS. The chapter will begin with a short discussion on the process used and the data created. This will be followed with the distinguishing features of the data created. Finally, a short discussion of the overall results and suggestions for future research are presented.

Summary

A FORTRAN program and Mathematica notebook were created and merged to a single tool that was used to manipulate data and build new data sets. The final version of these tools proved to be efficient in handling large data files of different sizes and processing the data they contained. New data files were created for each data set processed. The new data files included temporal profiles of event temperature, relative fractional FOV, RMSE for data processed at each time step, statistical values for each time step processed and intensity files representing profiles of an individual time step selected by the user. The code was created so future research efforts could manipulate the data differently with minimal changes to the code. The program was used to process over thirty data files in the course of this research.

Conclusions

The investigation of the derived data show identifiable features for different explosive species. Some data did not clearly display the anticipated features after processing. These anomalies appeared to be from differences in the parameters surrounding the event such as observation elevation, angle of attack and impact surface. In most of these cases the features were as expected but were not definite.

The resulting data created verified the description of detonation events as decaying graybodies. The data from large type B explosives consistently produced a clear afterburn feature. The fractional field of view for all type B events indicated a peak value corresponding with event initiation followed immediately by a distinct drop-off and steady value. Type A explosives showed an exponential decay of temperature from the peak value of initiation. The fractional field of view display for type A explosives showed a steady profile without an initial peak. The form of the RMSE generally showed the same time mode as its associated temperature profile. These observations indicate that event species can possibly be determined by temperature and/or fractional field of view profiles.

Discussion

The findings of this research indicate that the concept of reducing large spectroradiometic data files into data representing event temporal features may be a viable means of event classification. Future research could refine the transmittance profile creation and the curve-fitting procedures used to better accomplish these reductions.

The temporal evolution of the fractional field of view profiles may be verifiable using IR imagery corresponding to each event. IR imagery was collected during the Radiant Brass data acquisition. Comparing this IR imagery with the fractional field of view profiles may verify the results of this research effort.

Collection of a wider range of explosive events would provide a better data set.

Completion of analysis on all data already collected would also provide a better analysis.

The low angle of observation seemed to be the major factor in degradation of initial data confidence. An elevated viewing angle during future data collection opportunities may increase the value of data collected during future research.

The process of reversing the atmospheric absorption could possibly be accomplished much more accurately. The transmittance values created with PLEXUS appeared to overestimate the absorption of signal at certain frequencies. The product of this over estimation was transmissivity values lower than actual conditions. This caused overestimated values of adjusted scene spectral radiance from the atmospheric correction process. The PLEXUS software used user input of the parameters ambient temperature, path length, geographic location, time/date of measurement and path elevation as inputs to the MODTRAN model. Relative humidity, atmospheric pressure and percentage of CO₂ are inferred from other inputs. A better initiation of MODTRAN using actual values of pressure, humidity and CO₂ content would almost certainly provide a better atmospheric correction profile.

Finally, the curve-fitting process used in the FORTRAN program created could be improved. During program execution, the curve fitting process takes 1-4 seconds for each time step. Over 500 iterations were required to reach the final variable values.

TableCurve found better results in less than 20 iterations with a process taking tenths of a second on average. Better numerical method techniques would almost certainly provide better results.

•

Appendix A: FORTRAN Analysis Code

```
Capt William F. Bagby
        input and interoperation of ASCII data files
1
        6 Nov 00
1
        calculating, ver 4.05
1
MODULE global_data
        IMPLICIT NONE
        SAVE
                                                         ! Planck's constant!
        REAL, PARAMETER :: h=6.626E-34
                                                         ! Speed of Light in cm/sec
        REAL, PARAMETER :: c=2.9979E10
                                                         ! Boatman's constant
        REAL, PARAMETER:: k=1.38E-23
                                                         ! 2*h*c^2
        REAL, PARAMETER :: C1=1.2E-12
        REAL, PARAMETER :: C2=1.439
                                                         ! h*c/k
END MODULE global data
MODULE sgerror
        USE global_data
        IMPLICIT NONE
        CONTAINS
                SUBROUTINE
LEASTERROR(s1,bkav,i,fgss,tgss,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n1)
                        IMPLICIT NONE
                                                         ! Time step being evaluated
                        INTEGER, INTENT(IN) :: i
                                                         ! Intensities array
                        REAL, INTENT(IN) :: s1(:,:)
                        REAL, INTENT(IN) :: bkav(:,:)
                                                         ! avg background intensity
                                                         ! Estimated F value
                        REAL, INTENT(IN) :: fgss
                                                         ! Mean intensity vale at time step i
                        REAL, INTENT(IN) :: rmean
                                                         ! Estimated Temperature value
                        REAL, INTENT(IN) :: tgss
                                                         ! Root mean square error
                        REAL, INTENT(OUT) :: sqdev
                                                         ! r^2 (coefficient of determination)
                        REAL, INTENT(OUT) :: rsq
                                                         ! F statistic (MSR/MSE)
                        REAL, INTENT(OUT) :: Fstat
                                                         ! Mean Square Error
                        REAL, INTENT(OUT) :: MSE
                                                         ! Mean Square Regression
                        REAL, INTENT(OUT) :: MSR
                                                         ! Sum of Squares about Mean
                         REAL, INTENT(OUT) :: SSM
                                                         ! Sum of Squares due to Error
                         REAL, INTENT(OUT) :: SSE
                                                         ! Degrees of Freedom n-m
                         REAL:: DOF
                                                         ! Root Mean Square Error (Fit Std Error)
                         REAL:: RMSE
                                                         ! Planckian temporary values
                        REAL :: ss11,ss22,ss33
                                                         ! Input values of frequency and radiance
                         REAL:: wave, wave1
                                                         ! Temporary stats values
                         REAL :: diff,diffsum,diffsq
                         REAL:: meandiff, meandiffsq
                                                         ! Temporary stats values
                                                         ! Temporary stats values
                         REAL :: diffsumsq
                                                         ! Number of data points used
                        INTEGER::n,n1
                        INTEGER:: m
                                                         ! Number of variables to be fit (2)
                                                         ! counters used to step through frequencies
                        INTEGER :: j,nw
                 PRINT*, "i= ",i," tguess= ",tgss," fguess= ",fgss !!!, "T bomb= ",tsave ! record fguess at
time step i
                 PRINT*,"nw=",nw," rmean=",rmean
                                                         ! Number of variables to be fit (2)
                         m=2
                         n=0
                         diffsum=0
                         diffsq=0
                         diffsumsq=0
```

```
sqdev=0
                        MSE=0
                        RMSE=0
                        MSR=0
                        Fstat=0
                        meandiff=0
                        meandiffsq=0
                        SSE=0
                        SSM=0
                        DO i=1,nw
                                wave=s1(i,1)
                                                        ! Wave number
                                        ! wave1=PLEXUS corrected intensity-background intensity
                                wave1=s1(j,i)
                                IF (wavel .ne. 0) THEN
                                        wave1=s1(j,i)-bkav(j,2)
                                        ss11=(fgss) * (C1 * wave**3/(Exp(C2 * wave/tgss)-1))
                                                        ! plankian radiance value for T=tempguess
                                        ss33=wave1
                                                        ! value from PLEXUS corrected data
                                        n=n+1
                                        meandiff= ss33 - rmean ! difference from mean squared
                                ELSE IF (wave1 == 0) THEN
                                        ss22=0
                                        ss33=0
                                        meandiff= 0
                                                        ! difference from mean squared
                                END IF
                                diff= ss22 - ss33
                                                        ! difference between radiance values
                                diffsq=diff*diff
                                                        ! to be used as absolute RMS error
                                SSE=SSE+diffsq
                                                        ! cumulative SSE errors.
                                meandiffsq=meandiff*meandiff
                                                                ! diff from mean squared for
absolute RMS error
                                SSM=SSM+meandiffsq
                                                      ! cumulative SSE errors.
                        END DO
                        DOF=n-m
                        n1=n
                        MSE=SSE/DOF
                        RMSE=SQRT(MSE)
                        sadev=RMSE
                        MSR=(SSM-SSE)/(m-1)
                                                        ! Mean Square Regression
                        Fstat=MSR/MSE
                                                        ! F-statistic
                        rsq=1-SSE/SSM
                END SUBROUTINE LEASTERROR
END MODULE sqerror
Program inputdata
USE global data
USE sgerror
IMPLICIT NONE
INTEGER,PARAMETER :: in3=3,in1=1,in2=2
                                                       ! unit numbers for reading external files
INTEGER,PARAMETER:: out=10,out1=11,out2=12
                                                       ! unit numbers for writing external files
INTEGER,PARAMETER:: out3=13,out4=14,out5=15
                                                        ! unit numbers for writing external files
INTEGER,PARAMETER:: out6=16,out7=17,out8=18
                                                       ! unit numbers for writing external files
INTEGER,PARAMETER:: out9=19,out10=20,out11=21
                                                       ! unit numbers for writing external files
INTEGER,PARAMETER:: out12=22,out13=23,out14=19
                                                       ! unit numbers for writing external files
INTEGER:: iwn,it
                                                       ! wavenumber and time step iteration
counter
```

```
INTEGER :: nw,nw1,nt,nn
                                                           ! total bins (intensities, PLEXUS, time)
INTEGER :: ios,ios1,ioread
                                                           ! datafile read/write error flags
                                                           ! total number of commas and returns
INTEGER :: commas.crs
INTEGER :: n,i,j,j1,ji,jj1
                                                           ! integer counters for loops
INTEGER:: m,m1,nt1,z,FF,ii
                                                           ! integer counters for loops
INTEGER:: error
                                                           ! error code for input
INTEGER:: length,flag2,flag1
                                                           ! length of character string from first record
INTEGER :: add1,flag,tflag,Fflag
                                                           ! integers for calculating bin averages
INTEGER :: iter,iter1,nnn
                                                           ! integers for calculating bin averages
REAL, ALLOCATABLE :: s(:,:)
                                                           ! intensity data @ each time and wave#
REAL, ALLOCATABLE :: s1(:,:)
                                                           ! PLEXUS corrected intensity data
REAL, ALLOCATABLE :: T(:,:)
                                                           ! Raw data temperature array
REAL, ALLOCATABLE :: T1(:,:)
                                                           ! PLEXUS data temperature array
REAL, ALLOCATABLE :: TT(:.:)
                                                           ! Temperature vs. time data
REAL, ALLOCATABLE :: FT(:.:)
                                                           ! Event fraction of FIELD OF VIEW vs.
time data
REAL.ALLOCATABLE :: times(:)
                                                           ! time steps array
REAL, ALLOCATABLE :: wn(:)
                                                           ! wave number array
REAL, ALLOCATABLE :: trn(:,:)
                                                           ! transmittance values from PLEXUS
REAL, ALLOCATABLE :: trn1(:,:)
                                                           ! transmittance interpolated from PLEXUS
REAL,ALLOCATABLE :: SSM1(:,:)
                                                           ! Array of errors for each time step fit
REAL, ALLOCATABLE :: bkav(:,:)
                                                           ! avg background subtracted
REAL, ALLOCATABLE :: ss2(:)
                                                           ! holds timestep mean value
REAL, ALLOCATABLE :: ss3(:)
                                                           ! holds timestep bin mean value
REAL :: delt,delwn,deltp
                                                           ! time step size, wave number step size
REAL :: t11,t12,s11,s12,s13,s4,s5
                                                           ! temporary value holders for building arrays
REAL:: finalwn
                                                           ! calculated final wave number value
REAL :: temps,tmpF,lower,lowers
REAL :: p,p1,avg,mm
REAL :: tguess,fguess,bin1,bin2,bin3,test
REAL :: abin1,abin2,abin3,wave.stempo.rad
REAL :: sse,time !diffsum,diffsumtot,diffsumsq,diff,diffsq, various curve fitting reals
REAL:: abin1old,abin2old,abin3old,oldtguess,fguesstart,fguess1,mse,msr,ssm,r1,r1sum,rmean
REAL:: diffsqold,sqdev,delF,oldsq,fgup,sqdn,sqdv,squp,fgdn,fstat,fitsq,fitsqold!,fitsqdiff
REAL:: tguesstart,oldsq1,tgdn,tgup,tguess1,oldsqt,sqdnt,squpt,rsq,rsqold,rsqtemp!.rsqdiff
REAL :: rsqup,rsqdn,oldrsq,ambient,tsave,sqtold,bkval,valbk,binav,abin,launch,FicF,flow
CHARACTER:: firstchar
                                          ! temporary char to determine number of records
CHARACTER*100000 :: charstring
                                          ! temporary char to determine elements per record
CHARACTER :: charstring1
                                          ! temporary char to determine datafile size
CHARACTER*10 :: stringvar
                                          ! temporary char to determine datafile size
CHARACTER (LEN=1):: tempchar
                                          ! temporary char to determine datafile size
CHARACTER (LEN=40) :: infile.name.name1
                                                  ! input data files path and name
CHARACTER (LEN=40) :: outfile,outfile1,outfile2
                                                          ! names output files created
CHARACTER (LEN=40) :: outfile3,outfile4,outfile5! names output files created
CHARACTER (LEN=40) :: outfile6,outfile7,outfile8! names output files created
CHARACTER (LEN=40) :: outfile9.outfile10.outfile11
                                                          ! names output files created
CHARACTER (LEN=40) :: outfile12.outfile13.outfile14
                                                          ! names output files created
!!!!! PROMPT for and receive name and path of ASCII data file to be used
infile='d:\infile.txt'
OPEN (UNIT=2, FILE=infile,STATUS="OLD",IOSTAT=ios)
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), name
                                                          ! Location of ASCII Data File IN
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), name1
                                                          ! Location of ASCII Transmittance file
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile2
                                                          ! Interpolated Transmittance file
```

```
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile1
                                                          ! Intensity at selected timestep
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile
                                                          ! Interpolated PLEXUS applied data
                                                          ! Temps at selected timestep
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile4
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile5
                                                          ! Temps for all timesteps
                                                          ! Avg Temp vs. time
READ (UNIT=2.FMT='(A40)'.IOSTAT=ios), outfile6
                                                          ! F vs. Time
READ (UNIT=2.FMT='(A40)', IOSTAT=ios), outfile7
                                                          ! SSM vs. time
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile8
                                                          ! Binvalue vs. time
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile9
                                                          ! Timestep size
READ (UNIT=2,FMT=*,IOSTAT=ios), delt
                                                          ! Selected timestep location
READ (UNIT=2,FMT=*,IOSTAT=ios), ji
                                                          ! cutoff value for PLEXUS
READ (UNIT=2,FMT=*,IOSTAT=ios), lower
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile10
                                                          ! Average Background profile (outfile10)
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile11
                                                          ! adjusted data 1 time step
READ (UNIT=2,FMT='(A40)',IOSTAT=ios), outfile12
                                                          ! fit errors data listing;
name=TRIM(name)
name1=TRIM(name1)
outfile2=TRIM(outfile2)
outfile1=TRIM(outfile1)
outfile3=TRIM(outfile3)
outfile=TRIM(outfile)
outfile4=TRIM(outfile4)
outfile5=TRIM(outfile5)
outfile6=TRIM(outfile6)
outfile7=TRIM(outfile7)
outfile8=TRIM(outfile8)
outfile9=TRIM(outfile9)
outfile10=TRIM(outfile10)
outfile11=TRIM(outfile11)
outfile12=TRIM(outfile12)
CLOSE (UNIT=2)
PRINT *, "ASCII INPUT FILE; (name)= ",name
PRINT *, "PLEXUS INPUT FILE; (name1)= ",name1
PRINT *, "Interpolated PLEXUS File; (outfile2)= ",outfile2
PRINT *, "Intensities vs. wavenumber for 1 timestep file; (outfile1)= ",outfile1
PRINT *, "Output ASCII divided by PLEXUS tansmittance file; (outfile)= ",outfile
PRINT *, "Output temperature vs. wave number file for 1 timestep; (outfile4)= ",outfile4
PRINT *, "Output ASCII Temperature Data file; (outfile5)= ",outfile5
PRINT *, "Output Temperature vs. time file; (outfile6)= ",outfile6
PRINT *, "Output F vs. time file; (outfile7)= ",outfile7
PRINT *, "fit error vs. time file; (outfile8)= ",outfile8
PRINT *, "2400-2800 cm^-1 avg amplitude vs. time file; (outfile9)= ",outfile9
PRINT *, "Average Background profile (outfile10)= ",outfile10
PRINT *, "PLEXUS and Background adjusted data 1 time step (outfile11)= ",outfile11
PRINT *, "fit errors data listing; (outfile12)= ",outfile12
PRINT *, "Temporal Resolution, the size of the timestep; (delt)= ",delt
PRINT *, "Location for selected time step to be viewed=",jj
PRINT *, "Lower PLEXUS BOUNDS, or the cutoff for which wavenumbers values are used= ",lower
        ****** OPEN ASCII INPUT FILE
OPEN (UNIT=3, FILE=name, STATUS="OLD", IOSTAT=ios)
IF (ios==0) THEN
        GO TO 44
ENDIF
PRINT *, " "
```

```
PRINT *, "Unable to open data file, checF path and filename and try again"
PRINT *, "The file below has an invalid filename or path"
PRINT *, name
PRINT *. " "
PRINT *, "Press return to continue."
PRINT *, " "
READ*
GO TO 900
44 CONTINUE
crs=0
commas=0
n=0
nw=0
nt=0
                                               ! find dimensions of array
DO n=1,18888
        crs=crs+1
                                               ! counts the number of records in the data set
        IF (crs = 1) THEN
                READ (UNIT=3,FMT='(A1)',IOSTAT=ios), firstchar
                                               ! Test for end of file and exit loop
                SELECT CASE (ios)
                                               ! end of file, no more data
                        CASE (:-1)
                                GO TO 100
                                               ! error reading ASCII data
                        CASE (1:)
                                error = -2
                                PRINT *, "ERROR Reading ASCII DATA!!!"
                                GO TO 100
                END SELECT
        ELSE IF (crs == 1) THEN
                                               ! Test for commas seperating data entries and count
                READ (UNIT=3,FMT='(A100000)'), charstring
                                                                ! Read 1st record
                length=LEN(TRIM(charstring))
                                              ! eliminate excess blanF spaces in charstring
                                               ! calculate length of trimmed charstring
                DO i=1,length
                        IF (charstring(i:i) == ',') THEN
                                                               ! Count commas
                                commas=commas+1
                        END IF
                END DO
        END IF
END DO
100 Continue
nt=commas+1
nw=crs-1
PRINT *. " "
PRINT *, "ASCII file wavenumber bins, nw=",nw
                                                       ! number of records or wavenumber bins
                                                       ! number of columns or time steps
PRINT *, "ASCII file time step columns, nt=",nt
                                ! Use nt-1; first entry in each record is a wave number not intensity
nt1=nt-1
                                               ! Allocate size of intensities array
ALLOCATE (s(nw,nt))
                                               ! Allocate size of time step array
ALLOCATE (times(nt1))
ALLOCATE (wn(nw))
                                               ! Allocate size of wavenumber array
!!!!!!!!!! Create the 1-D timestep array !!!!!!!!
DO i=1,nt1
        times(i)=(i-1)*delt
END DO
CLOSE (UNIT=3)
```

```
OPEN (UNIT=3, FILE=name, STATUS="OLD", POSITION="REWIND", IOSTAT=ios)
!!!!!!!!!! Create the 2-D intensities array !!!!!!!
wn=0
DO i=1,nw
       READ (UNIT=3,FMT=*,IOSTAT=ioread)(s(i,j),j=1,nt)
       wn(i)=s(i,1)
       IF (ios/=0) THEN
               PRINT *, '("Error ",15,"while reading ",A)', name
       ENDIF
END DO
delwn=wn(2)-wn(1)
finalwn=delwn*nw
!!!! OPEN PLEXUS INPUT FILE
OPEN (UNIT=1, FILE=name1, STATUS="OLD", IOSTAT=ios)
IF (ios==0) THEN
       GO TO 45
ENDIF
PRINT *. " "
PRINT *, "Unable to open data file, checF path and filename and try again"
PRINT *, "The file below has an invalid filename or path"
PRINT *, name1
PRINT *, "Press return to continue."
READ*
GO TO 900
45 CONTINUE
crs=0
n=0
nw1=0
DO n=1,9888 ! Outer loop counts the number of records in the PLEXUS data set
       crs=crs+1
       IF (crs = 0) THEN
               READ (UNIT=1,FMT='(A1)',IOSTAT=ios), firstchar
                                            ! Test for end of file and exit loop
               SELECT CASE (ios)
                                                    ! end of file, no more data
                      CASE (:-1)
                              GO TO 110
                      CASE (1:)
                                                    ! error reading
                              error = -2
                              PRINT *, "ERROR Reading PLEXUS DATA!!!"
                              GO TO 110
               END SELECT
       END IF
END DO
110 CONTINUE
nw1=crs-1
PRINT *. " "
PRINT *, "PLEXUS wavenumber bins, nw1=",nw1
                                     ! Allocate size of origional PLEXUS array
ALLOCATE (trn(nw1,2))
                                     ! Allocate size of interpolated PLEXUS array
ALLOCATE (trn1(nw,2))
CLOSE (UNIT=1)
!!!!!!!!! Create the 2-D PLEXUS array !!!!!!!
OPEN (UNIT=1, FILE=name1, STATUS="OLD", POSITION="REWIND", IOSTAT=ios)
DO i=1,nw1
```

```
READ (UNIT=1,FMT=*,IOSTAT=ioread)(trn(i,j),j=1,2)
       IF (ios/=0) THEN
               PRINT *, "Error while reading ", name1
               GO TO 111
       ENDIF
END DO
111 CONTINUE
PRINT *. " "
CLOSE (UNIT=1)
!!! Create a new transmittance file with same wavenumber bins as the ASCII file (interpolated)
                                                                       ! Output interpolated
OPEN (UNIT=2,FILE=outfile2,STATUS="REPLACE",IOSTAT=ios1)
PLEXUS outfile2
                                                                       ! Selected step ASCII
OPEN (UNIT=11,FILE=outfile1,STATUS="REPLACE",IOSTAT=ios1)
Data outfile1
trn1=0
i=1
124 CONTINUE
IF (i > nw) THEN
        GOTO 123
END IF
s11=wn(i)
s12=s(i,ij)
                                               ! interpolated PLEXUS file
WRITE (UNIT=21,FMT=*) s11,s12
DO m=1,nw1
       IF (wn(i) \ge trn(m,1)) THEN
       m1=m+1
                IF (wn(i) < trn(m1,1)) THEN
                       t11=wn(i)
                        t12=(wn(i)-trn(m,1))*((trn(m1,2)-trn(m,2))/(trn(m1,1)-trn(m,1)))+trn(m,2)
                        trn1(i,1)=t11
                        trn1(i,2)=t12
                        WRITE (UNIT=21,FMT=*) trn1(i,1),trn1(i,2) ! Create interpolated File
                        i=i+1
                        GO TO 124
               ELSE IF (wn(i) \ge trn(m1,1)) THEN
                        CONTINUE
               END IF
        ELSE IF (wn(i) < trn(m,1)) THEN
                PRINT *, "I was here"
                GO TO 123
        END IF
END DO
123 CONTINUE
ENDFILE 21
CLOSE (UNIT=21)
ENDFILE 2
CLOSE (UNIT=2)
!!!! Divide the intensity by the transmittance to approximate original emittance
PLEXUS adjusted outfile
ALLOCATE (s1(nw,nt))
DO i=1,nw
        s1(i,1)=wn(i)
        DO j=2,nt
                IF (trn1(i,2) < lower) THEN
```

```
t11=0
                       s1(i,j)=t11
                ELSE IF (trn1(i,2) >= lower) THEN
                       t12=1/trn1(i,2)
                       t11 = t12 * s(i,j)
                       s1(i,j)=t11
                END IF
       END DO
END DO
                               ! array of all temps derived from Plexus corrected data
ALLOCATE (T1(nw,nt))
ALLOCATE (T(nw,2))
                               ! array of temps at selected time step
OPEN (UNIT=4,FILE=outfile4,STATUS="REPLACE",IOSTAT=ios1) !outfile4=Derived temps for 1
time step
lowers=.0000001
DO i=1,nw
               !! Create a derived temperature array
       t11=wn(i)
       t1(i,1)=t11
       DO FF=1.nt
                IF (ABS(s1(i,FF)) < lowers) THEN
                       t11=0
                       t1(i,FF)=t11
                ELSE IF (ABS(s1(i,FF)) >= lowers) THEN
                       IF (s1(i,FF) \ge 0.0) THEN
                               s4=ABS(s1(i,FF))
                               t11=(c * h * s1(i,1)) / (k)
                               t12 = \log(((2*h*c**2*(s1(i,1))**3)/(s4))+1)
                               flag1=1.0
                       ELSE IF (s1(i,FF) < 0.0) THEN
                               s4=ABS(s1(i,FF))
                               t11=(c * h * s1(i,1)) / (k)
                               t12 = \log(((2*h*c**2*(s1(i,1))**3)/(s4))+1)
                               flag1 = -1.0
                       END IF
                       t1(i,FF)=(flag1*(t11/t12))
                END IF
       END DO
                                               ! Temperatures from PLEXUS Corrected data
        WRITE (UNIT=4,FMT=*) wn(i),t1(i,jj)
END DO
ENDFILE 4
CLOSE (UNIT=4)
OPEN (UNIT=5,FILE=outfile5,STATUS="REPLACE",IOSTAT=ios1)! Out ASCII Temperature
Data=outfile5
DO i=1,nw
        WRITE (UNIT=5,FMT=*) (t1(i,j),j=1,nt) ! ASCII Temperature vs. wave# (all times)
ENDDO
ENDFILE 5
CLOSE (UNIT=5)
CLOSE (UNIT=3)
!!!!! CURVE FIT THE DATA TO MATCH A TEMPERATURE AND COEFFICIENT !!!!!!
ALLOCATE (bkav(nw,2))
ALLOCATE (ss2(nt1-1))
ALLOCATE (ss3(nt1-1))
ALLOCATE (TT(nt1-1,2))
ALLOCATE (FT(nt1-1,2))
ALLOCATE (SSM1(nt1-1,2))
```

```
bkval=0
valbk=0
FicF=.0000001
binay=0
tguess=1500
fguess=2
tflag=0
abin1old=10
ambient=300
flow=.02
iter=0
fguess1=fguess
tguess1=tguess
n=0
nn=0
bkav=0
abin=0
!outfile12="c:\errors.txt"
OPEN (UNIT=12,FILE=outfile12,STATUS="REPLACE",IOSTAT=ios1)! Out ASCII Temperature
Data=outfile5
WRITE (UNIT=12,FMT=*) "lower PLEXUS bounds=
                                                      ".lower
WRITE (UNIT=12,FMT=*) "ASCII INPUT FILE;
                                                    ",name
WRITE (UNIT=12,FMT=*) "PLEXUS INPUT FILE;
                                                      ",name1
WRITE (UNIT=12,FMT=*) "Interpolated PLEXUS File;
                                                     ",outfile2
WRITE (UNIT=12,FMT=*) "ASCII divided by PLEXUS file; ",outfile
WRITE (UNIT=12,FMT=*) "ASCII Temperature Data file; ",outfile5
WRITE (UNIT=12,FMT=*) "Temperature vs. time file; ",outfile6
WRITE (UNIT=12,FMT=*) "Fractional FIELD OF VIEW vs. time file; ",outfile7
                                                ",outfile8
WRITE (UNIT=12,FMT=*) "fit error vs. time file;
WRITE (UNIT=12,FMT=*) "2400-2800 cm^-1 avg vs. time; ",outfile9
WRITE (UNIT=12,FMT=*) "Temporal Resolution,
                                                   ".delt
WRITE (UNIT=12,FMT=*) " "
DO i=2,nt1
        rmean=0
        r1sum=0
        add1=0
        abin1=0
        bin1=0
!
        n=0
        DO j=1,nw
                r1=s1(i,2)
                r1sum=r1sum + r1
                                                               ! Bin 1 2400-2800 cm^-1
                IF (s1(j,i) .ne. 0) THEN
                        add1=add1+1
                        IF (s1(j,1) > 2400) THEN
                                IF (s1(j,1) < 2800) THEN
                                        bin1=bin1+s1(j,i)
                                        n=n+1
                                END IF ! (s1(j,1) < 2800)
                        END IF! (s1(j,1) > 2400) THEN
                END IF
        END DO! j=1,nw
        rmean=r1sum / add1
        abin1=bin1 / add1
```

```
ss2(i-1)=abin1
                                        ! average signal in 2400-2800 range at timestep i
        ss3(i-1)=rmean
                                        ! average signal at timestep i
        IF (i \ge 3) THEN
                IF (i < 12) THEN
                        binav=abin1+binav
                        nn=nn+1
                END IF
        END IF
END DO! i=2.nt1
binav=binav/nn
bkav=0
nnn=0
DO j=1,nw
        nnn=0
        DO i=3,12
                nnn=nnn+1
                IF (s1(j,i) .ne. 0) THEN
                        bkav(j,2)=s1(j,i)+bkav(j,2)
                ELSE IF (s1(i,i) == 0) THEN
                        bkav(j,2)=0
                END IF
        END DO
END DO
Print*,"add1=",add1
Print*,"nnn=",nnn
DO j=1,nw
        bkav(j,1)=s1(j,1)
        IF (bkav(j,2) .ne. 0) THEN
                bkav(j,2)=bkav(j,2)/nnn
        END IF
END DO
launch=0
OPEN (UNIT=11.FILE=outfile11.STATUS="REPLACE".IOSTAT=ios1)
OPEN (UNIT=10,FILE=outfile,STATUS="REPLACE",IOSTAT=ios1)
DO i=1.nw
        bkav(i,2)=bkav(i,2)
                                        !/add1
        bin1=s1(i,jj) - bkav(i,2)
        WRITE (UNIT=10,FMT=*) s1(i,1),bin1 ! PLEXUS And Bkgd Corrected 1 time step ji
        WRITE (UNIT=11,FMT=*) (bkav(i,j),j=1,2)
                                                        ! av bkd signal profile
ENDDO
ENDFILE 11
CLOSE (UNIT=11)
ENDFILE 10
CLOSE (UNIT=10)
DO i=2,nt1
        Fflag=0
        iter=0
        rsgold=1
        sqtold=0
        n=0
        rmean=ss3(i-1)
        test=ss2(i-1)
        IF (test <= 2.0 * binav) THEN
                                        ! check for a large increase in intensity
                tguess1=ambient
```

```
fguess1=0.0
                launch=0
                GO TO 446
        ELSE IF (test > 2.0 * binay) THEN! check for a large increase in intensity
                        (launch ==0) THEN
                IF
                        tguess1=1500
                        fguess1=2
                        launch=launch + 1
                END IF
442 Continue
                fguesstart=fguess1
                tguesstart=tguess1
                iter=0
                Fflag=Fflag+1
444 Continue
                flag=0
443 Continue
                iter=iter+1
                IF (iter == 120) THEN
                        PRint*, "I got out at line 527"
                        GO TO 446
                END IF
                delF=(.5 ** iter) * fguesstart
                                                         !find MSE at fguess
                CALL
LEASTERROR(s1,bkav,i,fguess1,tguess1,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                oldsq=sqdev
                oldrsq=rsq
                fgdn=fguess1-delF
                                                         !find MSE below fguess
                CALL
LEASTERROR(s1,bkav,i,fgdn,tguess1,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                sqdn=sqdev
                rsqdn=rsq
                                                         !find MSE above fguess
                fgup=fguess1+delF
                CALL
LEASTERROR(s1,bkav,i,fgup,tguess1,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                squp=sqdev
                rsqup=rsq
                IF (oldsq <= squp) THEN
                        IF (oldsq <= sqdn) THEN
                                fitsgold=oldsg
                                 GOTO 451
                        ELSE IF (oldsq > sqdn) THEN
                                IF (squp > sqdn) THEN
                                         fguess1=fgdn
                                         fitsgold=sqdn
                                         GOTO 451
                                END IF
                        END IF
                ELSE IF (oldsq > squp) THEN
                        fguess1=fgup
                        fitsqold=squp
                        GOTO 451
                END IF
```

```
451 CONTINUE
                deltp=(.5 ** iter) * tguesstart
                CALL
LEASTERROR(s1,bkav,i,fguess1,tguess1,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                oldsat=sadev
                rsqtemp=rsq
                                                                         !find MSE above Tguess
                tgdn=tguess1-deltp
                CALL
LEASTERROR(s1,bkav,i,fguess1,tgdn,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                sqdnt=sqdev
                rsqdn=rsq
                                                                         !find MSE below Tguess
                tgup=tguess1+deltp
                CALL
LEASTERROR(s1,bkav,i,fguess1,tgup,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)\\
                squpt=sqdev
                rsqup=rsq
                IF (oldsgT \leq squpT) THEN
                        IF (oldsqT \le sqdnT) THEN
                                                                 ! sadev is less than up or down step
                                IF (rsgold == rsgtemp) THEN
                                        IF (flag \geq 90) THEN
                                                GO TO 446
                                        ELSE IF (flag < 90) THEN
                                                Flag=flag+1
                                                rsgold=rsgtemp
                                                 go to 443
                                        END IF
                                ELSE IF (rsgold .ne. rsgtemp) THEN
                                        rsgold=rsgtemp
                                        IF (1 <= Fflag) THEN
                                                IF (Fflag <= 75) THEN
                                                         GO TO 442
                                                END IF
                                        END IF
                                        GO TO 444
                                END IF
                        ELSE IF (oldsqT > sqdnT) THEN
                                                                 ! sqdev is less than up or down step
                                IF (squpt > sqdnt) THEN
                                        tguess1=tgdn
                                        rsqold=rsqdn
                                        IF (1 <= Fflag) THEN
                                                IF (Fflag <= 75) THEN
                                                         GO TO 442
                                                END IF
                                        END IF
                                        GO TO 444
                                END IF
                        END IF
                ELSE IF (oldsqt > squpt) THEN
                        tguess1=tgup
                        rsqold=rsqup
                        IF (1 <= Fflag) THEN
```

```
IF (Fflag <= 75) THEN
                                       GO TO 442
                               END IF
                       END IF
                        GO TO 444
                END IF
       END IF ! (ss2(i-1) <= 1.5 * binav)
446 CONTINUE
       fguess=fguess1
       tguess=tguess1
       fitsa=oldsat
       time=i*delt
       If (launch .ne. 0) THEN
                Print*.""
                CALL
LEASTERROR(s1,bkav,i,fguess,tguess,nw,sqdev,rsq,fstat,mse,msr,ssm,rmean,sse,n)
                Print*, "step i=",i," at time=",time," after",iter," iterations"
                PRINT*, "fguess= ",fguess," tguess= ",tguess !!!, "T bomb= ",tsave
                                                                               ! record fguess at
time step i
                PRINT*, "SSE=", SSE," SSM=", SSM," nw=",nw
                PRINT*,"MSR=",MSR," MSE=",MSE," RMSE=",sqdev
                PRINT*, "Fstat=",fstat," rsq=",rsq," n=",n
                WRITE (UNIT=12,FMT=*)""
                WRITE (UNIT=12,FMT=*)"step i=",i," at time=",time," after",iter," iterations"
                WRITE (UNIT=12,FMT=*)"fguess= ",fguess," tguess= ",tguess !!!,"T bomb= ",tsave
        ! record fguess at time step i
                WRITE (UNIT=12,FMT=*)"SSE=",SSE," SSM=",SSM," nw=",nw
                WRITE (UNIT=12,FMT=*)"MSR=",MSR," MSE=",MSE," RMSE=",sqdev
                WRITE (UNIT=12,FMT=*)"Fstat=",fstat," rsq=",rsq," n=",n
        END IF
        TT(i-1,1)=times(i-1)
                                ! Create timestep
                                ! Temperature converted in Kelvin
        TT(i-1,2)=tguess
        FT(i-1,1)=times(i-1)
        FT(i-1,2)=fguess! FIELD OF VIEW Fraction guess
        SSM1(i-1,1)=times(i-1)
        SSM1(i-1,2)=sqdev
                                        ! error guess
               ! i
END DO
!!! Create temperature for each time step file
OPEN (UNIT=6,FILE=outfile6,STATUS="REPLACE",IOSTAT=ios1) ! Out ASCII Temp vs. time
=outfile6
OPEN (UNIT=7,FILE=outfile7,STATUS="REPLACE",IOSTAT=ios1) ! Out ASCII F vs. time =outfile7
OPEN (UNIT=8,FILE=outfile8,STATUS="REPLACE",IOSTAT=ios1)
                                                                       ! Out ASCII fit errors
DO ii=1.nt1-1
        WRITE (UNIT=6,FMT=*) (TT(ji,j),j=1,2)
                                                       ! Temperature vs. time in K
        WRITE (UNIT=7,FMT=*) (FT(jj,j),j=1,2)
                                                       ! FIELD OF VIEW Fraction guess vs. time
        WRITE (UNIT=8,FMT=*) (SSM1(jj,j),j=1,2)
                                                       ! error guess vs. time
ENDDO!ii
ENDFILE 6
CLOSE (UNIT=6)
ENDFILE 7
CLOSE (UNIT=7)
ENDFILE 8
CLOSE (UNIT=8)
ENDFILE 12
```

CLOSE (UNIT=12) 900 CONTINUE END Program inputdata

Appendix B: Mathematica Analysis Code

This is a sample Mathematica notebook used to create an IO file for the FORTRAN code and then execute the program. Below the Run["c:\prog.exe"] command are commands developed to display the contents of the data files built during program execution. During data processing two of these notebook scripts were created, one for the A sensor on the instrument and the other for the B sensor.

```
<< Graphics`MultipleListPlot`
h = 6.626*10^{(-34)}; c = 2.9979*10^{10}; k = 1.38*10^{(-23)};
T1 = 300; T2 = 873; T3 = 1073; T4 = 1173; T5 = 1273;
 S[\lambda , T] := ((10^16/[\lambda]^5)*((2*h*c^2)/((Exp[(1000*c*h)/(\lambda*k*T)] - 1)))
                                    (* Frequency Planck curve *)
 S1[\sigma_{-}, T_{-}] := (2*h*c^2*[\sigma]^3)/((Exp[(c*h*[\sigma])/(k*T)] - 1))
                                   (* Wave Number Planck curve *)
TT[S\_\sigma_] := (c*h*[\sigma])/(k*Log[(2*h*c^2*[\sigma]^3)/S + 1]))
                                    (* Inverse Planck to get Temperature *) )))
list5 = Table[\{j, S1[j, 1100]\}, \{j, 2, 5990, 2\}\}; (* 1100K Curve *)
                                   (* Transmissivity file *)
trns = ReadList[var2a, {Number, Number}];
ListPlot[list5, Axes -> True, ImageSize -> 400, Frame -> True,
FrameLabel -> {"Wavenumber (cm^-1)", "Radiance", "For 1100 K", " " }]
ListPlot[trns, ImageSize -> 400, Axes -> True, Frame -> True,
 FrameLabel -> {"Wavenumber (cm^-1)", "Transmittance", "PLEXUS", var2a }]
                          (* 300 K curve times transmittance from plexus *)
comp1 = Table[\{2*j + 396, (list5[[j + 199, 2]]*trns[[j, 2]])\}, \{j, 2, 2800, 2\}\};
                          (* Now set limits for same wavenumber outputs *)
ListPlot[comp1, Axes -> True, ImageSize -> 400, Frame -> True, PlotJoined -> True, PlotRange -> {{-200,
6000}, {-.00002, .00078}}, FrameLabel -> {"Wavenumber (cm^-1)", "Spectral Radiance (W/cm^2 sr cm^-
1)", "1100 K", ""}]
(* Define Location of input intensities ASCII File to be used *)
                 var1a = "d:Big1a.txt";
(* Define Location of input PLEXUS Transmittance File to be used *)
                 var2a = "c:big1.trn";
(* Define Location for output interpolated PLEXUS Transmittance File *)
                 var3a = "d:TempNewtrn_a.trn";
(* Define Location for output Temperatures at all timesteps data *)
                 var7a = "d:TempTcube_a.txt";
```

```
(* Define Location for output average temperature vs. time data *)
                 var8a = "d:TempTemptime a.txt";
(* Define Location for output average F vs. time data *)
                 var9a = "d:TempFtime_a.txt";
(* Define Location for output error vs. time data *)
                 var10a = "d:Temperrortime_a.txt";
(* Define Location for output average 2400 - 2800 cm^-1 value vs. time data *)
                 var11a = "d:Tempbinvaltime_a.txt";
(* Define time step size in seconds *)
                 delt = .0454;
(* Define Location for fit errors and statistics *)
                 var14a = "d:TempFitErrora.txt";
(* Define Location for output Avg bkgd profile *)
                 var12a = "d:Tempavbacka.txt";
(* Define data step number to be used for instantaneous values *)
                 step = 41;
(* Define Location for raw output intensity at 1 time step *)
                 var4a = "c:dataE98 03aRaw42a.txt";
(* output iterpolated PLEXUS applied data at 1 time step *)
                 var5a = "c:dataE98 03aPlex42a.txt";
(* PLEXUS and background adjusted data at 1 timestep *)
                 var13a = "d:adidata42a.txt":
(* Define Location for output Temperatures at 1 timestep *)
                 var6a = "d:Temps42a.txt";
(* Define lower bounds of PLEXUS to be used; (Cutoff) *)
                 bounds = .4:
var1 = OutputForm[var1a]; var2 = OutputForm[var2a]; var3 = OutputForm[var3a];
var4=OutputForm[var4a]; var5 = OutputForm[var5a]; var6 = OutputForm[var6a];
var7=OutputForm[var7a]; var8 = OutputForm[var8a]; var9=OutputForm[var9a];
var10=OutputForm[var10a]; var11=OutputForm[var11a]; var12 = OutputForm[var12a];
var13=OutputForm[var13a]; var14 = OutputForm[var14a];
Put[var1, var2, var3, var4, var5, var6, var7, var8, var9, var10, var11, delt, step, bounds, var12, var13,
var14, "d:infile.txt"]
Run["d:prog.exe"];
tstep = step*delt;
(* raw data at one timestep *)
data2 = ReadList[var4a, {Number, Number}];
ListPlot[data2, Axes -> True, ImageSize -> 400, Frame -> True,
 PlotRange \rightarrow {{0, 6000}, {-.0001, .0012}},
 FrameLabel -> {"Wavenumber (cm^-1)",
    "Scene Spectral Radiance (W/cm^2 sr cm^-1)", "HgCdTe Raw Data", ""}]
(* PLEXUS Corrected raw data at one time step *)
corr = ReadList[var5a, {Number, Number}];
ListPlot[corr, Axes -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{0,6000}, {-0.0001,
.007}}, FrameLabel -> {"Wavenumber (cm^-1)", "Scene Spectral Radiance (W/cm^2 sr cm^-1)",
"HgCdTe Corrected Data", " " }]
(* Temperatures from raw data in FORTRAN *)
temps = ReadList[var6a, {Number, Number}];
ListPlot[temps, Axes -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{0,6000}, {-3000,
3000}}, FrameLabel -> {"Wavenumber (cm^-1)", "Temperature (Kelvin)", var6a, tstep}]
```

```
(* Temperature vs. time *)
temps = ReadList[var8a, {Number, Number}];
ListPlot[temps, Axes -> True, PlotJoined -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{1,
4}, {-100, 1650}}, FrameLabel -> {"Time (sec)", "Temperature (K)", var8a, bounds }]
(* K vs. time *)
temps = ReadList[var9a, {Number, Number}]; ListPlot[temps, Axes -> True, PlotJoined -> True,
ImageSize -> 400. Frame -> True, PlotRange -> {{1, 4}, {-.1, 15}}, FrameLabel -> {"Time (sec)", "F",
var9a, bounds \]
(* average background radiance *)
bkav = ReadList["c:bkav.txt", {Number, Number}];
ListPlot[bkav, Axes -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{000, 6050}, {-.0001,
.0003}}. FrameLabel -> {"Time (sec)", "Scene Spectral Radiance (W/cm^2 sr cm^-1)", "HgCdTe
Average Background Signal", "" }]
(* 2400 - 2800 cm^-1 avg vs. time *)
temps = ReadList[var11a, {Number, Number}]:
ListPlot[temps, Axes -> True, PlotJoined -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{-
0.10, 11}, {-.001, .004}}, FrameLabel -> {"2400-2800 cm^-1 avg", "bin average", var11a, bounds }]
(* error vs. time *)
temps = ReadList[var10a, {Number, Number}];
ListPlot[temps, Axes -> True, PlotJoined -> True, ImageSize -> 400, Frame -> True, PlotRange -> {{-
0.10, 11}, {-0.0000001, .0009}}, FrameLabel -> {"2400-2800 cm^-1 avg", "error", var10a, bounds }]
```

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Vita

Captain William F. Bagby was born on in Denver, Colorado.

He graduated from Alameda High School Lakewood, CO in June of 1984. He enlisted in the United States Air Force on 18 March 1986 as an instrumentation Mechanic Apprentice. During his enlistment he was stationed at Hill Air Force Base, Utah and the United States Air Force Academy, Colorado. In September of 1991 he received an Associate of Applied Science in Electronic Systems Technology from the Community College of the Air Force. While stationed at the USAFA, he was selected to finish his undergraduate studies through the Airman's Education and Commissioning Program (AECP). He completed his undergraduate studies at the University of Utah in June of 1996. He graduated Magna Cum Laude receiving a Bachelor of Science Degree in Meteorology with a Mathematics minor.

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The remote observations of the temporal and spectral characteristics of the infrared (IR) emissions from exploding ordnance have been correlated with explosion conditions. A Bomem MR-154 Fourier Transform Interferometer with two detectors, InSb and HgCdTe, was used to record spectra in the 1.3 - 20 µm range. Data was collected at spectral resolutions of 16 cm ⁻¹ and 4 cm ⁻¹ , and temporal resolutions of 0.045 s and 0.123 s, respectively. The data files range in size from 900 Kilobytes to several Megabytes. These are reduced to 2-dimensional representations of temporal features that are less than 100 Kilobytes.								
The data analysis indicates the possibility of characterizing event species through one or more derived temporal features. Each event data matrix contains three dimensions of information describing radiance as a function of frequency and time. The observed data is first corrected for atmospheric losses to convert apparent radiance to emitted radiance. The data is then adjusted to remove background radiance. Finally, the corrected data is fit to a Planckian distribution function to compute event temperature and fractional field of view. Temporal profiles of temperature and fractional field of view are created to describe each event. The temporal profiles of each explosive type are compared to other explosive types. Certain explosive types indicated an afterburn feature on their temperature profiles. The afterburn feature wasn't apparent on the temperature profiles of other types. Additionally, the temporal evolution of fractional field of view was unique for each explosive type.								
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